“Nicolae Testemițanu” State University of Medicine and Pharmacy
Moldova State University
Institute of Chemistry of MSU
Institute of Mother and Child

International Congress
MEDICINE, MOLECULAR AND ENVIRONMENTAL SCIENCES 2025

“From chemistry to medicine – 35 years of Moldo-Romanian scientific collaboration”

BOOK OF ABSTRACTS

November, 10-15 2025
Chișinău, Republic of Moldova

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WELCOME

We are delighted to welcome you at the International Congress "MEDICINE, MOLECULAR AND ENVIRONMENTAL SCIENCES 2025" in Chisinau and we thank you for attending.

Please join us in celebrating 35 years of Moldo-Romanian scientific collaboration.

The MedMolMed 2025 congress aims to play a key role in developing research and expanding collaboration in the fields of molecular and life sciences. Expanding collaboration between scientists from Moldova and Romania is essential for maintaining our relevance, competitiveness, and visibility in the European and global academic area.

Topics include basic and applied researches as well as case studies in the fields of medicine, chemistry, physics and all related biomedical and molecular areas (pharmacy, biochemistry, food sciences, material sciences, crystal engineering, ecology, etc).

There are over 350 registered participants and over 200 papers presented in MedMolMed 2025. We thank you for the interest shown in this event.

Last but not least, we wish to thank all the sponsors and institutions for their commitment and much appreciated support of the conference. We hope that direct contacts btween sponsors and participants will enhance collaboration in future reserch projects and infrastructure development.

We hope that the program will stimulate enthusiastic discussions and we wish you a nice stay in Chisinau.

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DIALOGUE-DEBATE

DEBATE1

The Truth in Science, Philosophy, Religion and Common Sense

Mircea Dumitru[1,2], Daniel David[1,3,4]

[1] Romanian Academy, Bucharest, Romania.
[2] University of Bucharest, Romania.
[3] Babeş-Bolyai University, Cluj-Napoca, Romania.
[4] Ministry of Education and Research, Bucharest, Romania.

A two-hours long public dialog, debating the concept of Truth from various perspectives. The starting point of the debate is the assessment that the development of the human society up to the current level was driven by the continuous search for knowledge and truth.

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PLENARY LECTURES

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PL1

Chemistry-pathology interface: uremic toxins and the risk in patients with chronic kidney disease

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Chronic kidney disease (CKD) is a global health burden that affects over 10% of the global population [1], with projections indicating that this progressive condition will be the 5th leading cause of death by the year 2040 [2]. Apart from traditional risk factors, such as diabetes mellitus and hypertension, elevated circulating metabolites, known as uremic toxins, accelerate adverse related outcomes. Uremic toxins are by-products or waste substances from dietary intake, gastrointestinal tract, and liver, that enter the bloodstream and are subsequently transported to the kidneys for filtration and removal from the body in the urine [3]. In CKD, the effective removal of these toxins is compromised, and even if uremic toxins are not fully known, it is well established that they progressively increase in CKD, promoting several functional changes. In this context, their accumulation is a key challenge in CKD management. Uremic toxins are classified based on their molecular weight, physicochemical properties, binding properties, and behavior during dialysis: small-molecule toxins (asymmetric dimethylarginine, trimethylamine N-oxide), middle molecule toxins, (β2-microglobulin, fibroblast growth factor 23, tumor necrosis factor-α) and protein-bound uremic toxins (indoxyl sulfate, p-cresol sulfate, advanced glycation end-products) [4]. Uremic toxins display a wide array of physicochemical characteristics, mechanisms of production, and pathobiological actions at both cellular and molecular levels [5]. The complexity of uremic toxins and their varying clearance rates across different dialysis modalities poses significant challenges, thus, a precise understanding of the uremic toxins features would be very useful in the design of strategies for their removal (by dialysis) and in the prevention or inhibition of their undesirable effects on tissues and organs. This paper explores recent advances in the qualitative and quantitative analysis of uremic toxins and highlights the use of innovative methods and integration of multiple disciplines that will provide deeper understanding of uremic toxin profiling and offer insights for improving hemodialysis programs.

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References

1. GBD Chronic Kidney Disease Collaboration. Lancet. 2020; 395(10225): 709-733. doi:10.1016/S0140-6736(20)30045-3.
2. Foreman KJ, Marquez N, Dolgert A, et al. Lancet. 2018;3 92(10159): 2052-2090. doi:10.1016/S0140-6736(18)31694-5.
3. Dalpathadu H, Salim AM, Wade A, Greenway, SC. Toxins 2024; 16: 345. doi: 10.3390/toxins16080345.
4. Cozzolino M, Magagnoli L, Ciceri P. Toxins (Basel). 2025;17(6):295. doi:10.3390/toxins17060295.
5. Falconi CA, Junho CVDC, Fogaça-Ruiz F, et al. Front Physiol. 2021; 12:686249. doi:10.3389/fphys.2021.686249.

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PL2

Multitarget azaheterocycles for anticancer and antimicrobial diseases

Violeta Mangalagiu[2], Gheorghita Zbancioc[1], Costel Moldoveanu[1], Dorina Amariucai-Mantu[1], Vasilichia Antoci[1], Ramona Danac[1], Ionel I. Mangalagiu[1]

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Cancer and microbial illness are multifactorial diseases difficult to treat with drugs that act on a single target [1-4]. Currently, there are two strategies to design the multi-targeting therapeutics. The first strategy, the classical one, consist in combinations of different drugs that interact with different single targets. The second strategy is to design and develop Multiple Targeting Drugs (MTD) where a single chemical entity interacts with two or more distinct biological targets related to a disease. The MTD drugs are usually classified in Hybrid Drugs (HD) and Chimeric Drugs (CD) [1-6]. The HD are designed by the Molecular Hybridization Technique (MHT), wherein two or more drug pharmacophores with different biological activities are connected via a flexible linker resulting in a single chemical entity. The CD are designed by merging or fusing the pharmacophores of two different drugs in a single chemical entity using an appropriate core.

As part of our continuous efforts in the field of azaheterocyclic derivatives, we present herein recent results obtained by our group in the field of multitarget azaheterocycles for anticancer and antimicrobial diseases [4-11]. The presentation will be focused on the design, synthesis, and biological activity of some hybrid and chimeric azaheterocyclic MTD derivatives. The antimicrobial and anticancer activity of azaheterocyclic derivatives will be presented, some of the compounds having excellent biological activity. Some of the obtained compounds are promising leading drug candidates.

References

1. Rodrig, D.A. Curr. Top. Med. Chem. 2022, 22, 331.
2. Ivasiv, V.; Albertini, C.; Goncalves, A.E.; Rossi, M.; Bolognesi, M.L. Curr. Top. Med. Chem. 2019, 19, 1694-1711.
3. Raghavendra, N.M.; Pingili, D.; Kadasi, S.; Mettu, A.; Prasad, S.V.U.M. Eur. J. Med. Chem. 2018, 143, 1277-1300.
4. Diaconu, D.; Savu, M.; Ciobannu, C.; Mangalagiu, V.; Mangalagiu, I.I. Bioorg. Med. Chem. 2025, 119, 118069.
5. Amariucai-Mantu, D.; Mangalagiu, V.; Bejan, I.; Aricu, A.; Mangalagiu, I.I. Pharmaceutics 2022, 14, 2026.
6. Lungu, C.N.; Bratanovici, B.I.; Grigore, M.M.; Antoci, V.; Mangalagiu I.I. Curr. Med. Chem. 2020, 27(1), 154-169.
7. Antoci, V.; Oniciuc, L.; Amariucai-Mantu, D.; Moldoveanu, C.; Mangalagiu, V.; Amarandei, A.M.; Lungu, C.N.; Dunca, S.; Mangalagiu, I.I.; Zbancioc, G. Pharmaceuticals 2021, 14, 335.
8. Popovici L., Amarandei R.M., Mangalagiu I.I., Mangalagiu V., Danac, R. J. Enzyme Inhib. Med. Chem. 2019, 34, 230-243.
9. Olaru A., Vasilache V., Danac R., Mangalagiu I.I. J. Enzyme Inhib. Med. Chem. 2017, 32, 1291-1298.
10. Luca, M.C, Tura, V; Mangalagiu I.I. Med. Hyp. 2010, 75, 627-629.
11. Zbancioc G., Bejan, V., Risca M., Moldoveanu, C., Mangalagiu I.I. Molecules 2009, 14, 403-411

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PL3

Design of molecules with strong anticancer properties

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- There are more than thirty years after the first approval of cis-platin in the clinic against a number of cancer diseases.
- Cisplatin and related compounds continue to be among the most efficient anticancer drugs used so far.
- Efforts are now focused to develop novel platinum- and non-platinum-based antitumor drugs to improve clinical effectiveness, to reduce general toxicity and to broaden the spectrum of activity.
- DNA is a main target for the therapeutic treatment of various disorders and diseases. It can interact with many biomolecules and synthetic compounds, including:
  - ✓ Alkilants agents
  - ✓ Intercalants agents
  - ✓ Antimetabolits agents
  - ✓ Immunosuppressers agents
- As summarized and illustrated above, the design and development of DNA-binding metal-containing drugs, requires detailed coordination-chemistry knowledge of the M-DNA binding processes, regarding structure, thermodynamics and kinetics. During the last decade, others and we have been giving attention to new approaches, like bifunctionality. This approach had started with attention to hydrogen bonding as a secondary interaction, and has developed towards attached intercalators, attached co-drugs and a second (or third) metal, all with a major aim to avoid resistance development or synthesis of tumour-specific drugs.

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PL4

Molecular diversity of ionic liquids: preparation of novel scaffolds and focused targets

Fliur Macaev

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Some examples for the strategic use of room-temperature liquid salts transformations will be discussed that enable efficient, flexible and straightforward synthesis of structurally demanding products of biological significance [1-7]. Particular focus will be on application of tunable nature of ionic compounds for formation metal-ion-containing ionic liquids, catalysts for the removal of pollutants, on a newly discovered example of double 6-exo-trig heterocyclization via nitrile conversion to new anticancer active primary amine ionic liquids. This communication arises from collaboration between Laboratory of organic synthesis, Institute of Chemistry, Moldova State University (Chișinău, Moldova) and Interdisciplinary Research Department, "Alexandru Ioan Cuza" University (Iasi, Romania).

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References

1. Macaev F. Green chemistry protocols: specific ionic liquids as recyclable reagents, catalysts, solvents and extractors. In: «Environmental Security Assessment and Management of Obsolete Pesticides in Southeast Europe», Eds. L. Simeonov, F. Macaev and B. Simeonova, SPRINGER Science+Business media B.V. Amsterdam, Dordrecht. 2013, p. 313-331. ISBN 978-94-007-6460-6.
2. Prodius, D.; Macaev, F.; Lan Y., Novitchi, G.; Pogrebnoi, S.; Stingaci, E.; Mereacre, V.; Anson, C. E.; Powell, A. K. Chemical Communications. 2013, 49, 9215-9217.
3. Prodius, D.; Macaev, F.; Stingaci, E.; Pogrebnoi, V.; Mereacre, V.; Novitchi, G.; Kostakis, G. E.; Anson, C. E.; Powell, A. K. Chemical Communications. 2013, 49 (19), 1915-1917.
4. Neamțu, M.; Macaev, F.; Boldescu, V.; Hodoroaba, V.D.; Nădejde, C.; Schneider, R. J.; Paul, A.; Ababei, G.; Panne, U. Applied Catalysis B: Environmental. 2016, 183, 335-342.
5. Boldescu, V.; Sucman, N.; Hassan, S.; Iqbal, J.; Neamtu, M.; Lecka, J.; Sévigny, J.; Prodius, D.; Macaev, F. ChemMedChem, 2018, 13, 2297-2304.
6. Pogrebnoi, S. Radul, O., Stingaci, E., Lupascu, L., Valica, V., Uncu, L., Smetanscaia, A., Petrou, A., Ciric, A., Glamoclija, J., Sokovic, M., Geronikaki, A. Macaev, F. Z. Anthibiotics 2022,*11*(5), 588.
7. Sucman, N.S., Bilan, D.YA., Cojocari, S.V., Pogrebnoi, V.S., Stîngaci, E.P., Khripach, V.A., Zhabinskii, V.N., Tsybruk, T.V., Grabovec, I.P., Panibrat, O.V., Persoons, L., Schols, D., Froeyen, M., Shova, S., De Jonghe, S., Macaev, F.Z. Steroids, 2024, 210, 109475

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PL5

Nature to nano: the hidden role of cellulose in bioelectronics for personalized medicine

Sergiu Coseri

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The rapid expansion of the bioelectronics sector has ushered in a new generation of functional devices capable of seamlessly interfacing with biological systems. From wearable sensors to implantable neural probes, the demand for materials that are flexible, biocompatible, sustainable, and electrically conductive has never been greater [1]. Conventional electronic materials—often based on rigid synthetic polymers or scarce metals—struggle to meet these requirements, particularly with respect to long-term environmental and biomedical compatibility. This limitation has spurred the search for bio-derived alternatives, with cellulose nanofibers (CNFs) emerging as one of the most promising candidates [2,3]. These CNFs combine high mechanical strength, large surface area, tunable surface chemistry, and optical transparency, making them versatile building blocks for next-generation bioelectronic devices. They can be processed into flexible films, aerogels, hydrogels, and composite structures, enabling integration into diverse device architectures [4]. Beyond their mechanical and environmental advantages, CNFs possess intrinsic features highly relevant to bioelectronics. Their hydrophilic and porous nature supports intimate interaction with cells, tissues, and ionic environments—an essential criterion for stable bioelectronic interfaces. Moreover, CNFs can be chemically modified or combined with conductive polymers, nanoparticles, or carbon-based nanomaterials to impart electronic conductivity without compromising their inherent sustainability and biocompatibility. Recent advances in wearable sensors, biodegradable electrodes, ion-conducting membranes, and implantable devices highlight the broad technological potential of CNF-based substrates. The transformative potential of CNFs lies in their ability to turn an ancient natural resource into cutting-edge technological solutions. By bridging the gap between biological systems and electronics, they represent a paradigm shift in material design—merging sustainability with high performance. This presentation examines the progress, challenges, and future opportunities of CNFs in bioelectronics, emphasizing their role in shaping the next generation of sustainable electronic technologies.

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References

1. Yao X., Zhang S., Wei N., Qian L., Coseri S. Cellulose-Based Conductive Hydrogels for Emerging Intelligent Sensors, Adv. Fiber Mater., 6, 1256–1305, 2024.
2. Yao X., Zhang S., Qian L., Wei N., Nica V., Coseri S., Han F. Super Stretchable, Self-Healing, Adhesive Ionic Conductive Hydrogels Based on Tailor-Made Ionic Liquid for High-Performance Strain Sensors, Adv. Funct. Mater., 32, 2204565, 2022.
3. Biliuta G., Coseri S. Coord. Chem. Rev., 383, 155-173, 2019.
4. Biliuta G., Dascalu A., Stoica I., Baron R. I., Bejan D., Bercea M., Coseri S. Structural and rheological insights of oxidized cellulose nanofibers in aqueous suspensions, Wood Sci. Technol., 57, 1443–1465, 2023.

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PL6

Building form and function of terpenoids: the new age of free radical chemistry

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[3]*Teva Pharmaceuticals SRL, Bucharest, Romania.*

Terpenes represent an enormous family of natural compounds with an impressive diversity of both carbon backbones and functionalization pattern. It is well known that this diversity is due to the last steps of terpene biosynthesis, comprising cyclizations, skeletal rearrangements and functionalization with heteroatoms. The known biosynthetic processes have inspired organic chemists to devise synthetic methods which selectively transform the substrates exactly in the same way as enzymes do, that is in a biomimetic manner. The current work presents application of this strategy for the late-stage molecular editing of natural terpenoids *via* C-C bond formation and functionalization of inactivated C-H bonds with heteroatoms. Following the biomimetic approach, the different free radical processes have been applied in order to integrate into terpenic structures an array of functional groups like hydroxy-, halo-, azide, amine, ester, lactam, pyrrolidine, guanidine and other functionalities (Figure 1).

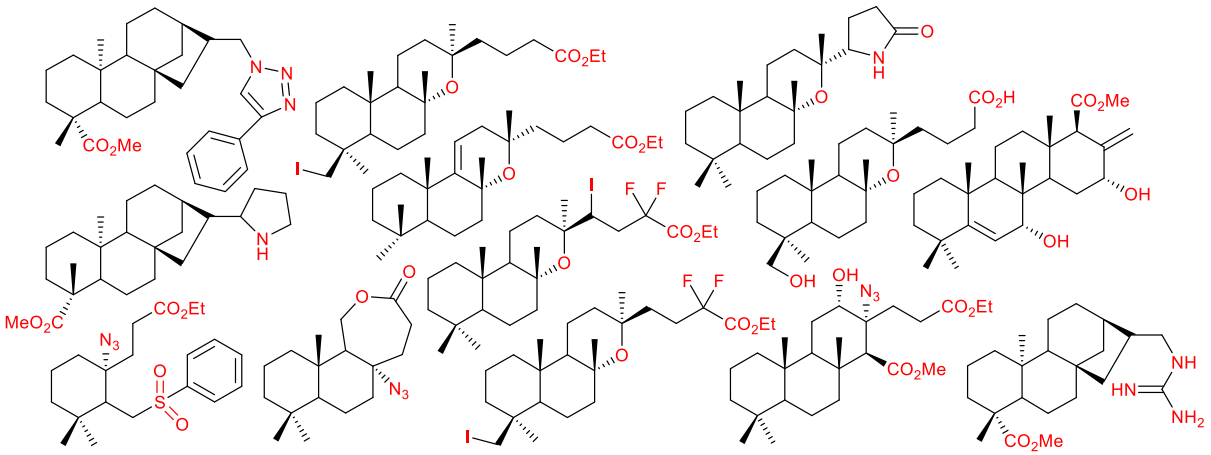

Figure 1. Terpenic compounds obtained synthetically by free radical transformations.

The advent of photo-redox catalysis with visible light provided an additional boost to these investigations, ensuring environmentally friendly processes and increased atom economy. The derived new compounds have been submitted to diverse biological assays and showed selective cytotoxicity against tumors, antimicrobial activity, as well as synergistic action with known antibiotics.

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PL7

Polysaccharide based (bio)hybrid nanostructures

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[2] Theoretical and Physical Chemistry Institute, Athens, Greece.

The results presented herein focuses on the synthesis of novel polymeric nanomaterials of natural polysaccharides covalently functionalized by synthetic, water soluble, responsive and biocompatible or biorelevant polymers. Reversible Addition Fragmentation Chain Transfer (RAFT) polymerization process was chosen as controlled radical polymerization technique to facilitate the attachment of functional polymer chains on polysaccharide chains, by grafting from or grafting to synthetic schemes, creating hybrid synthetic-biological polymers of advanced functionality and properties [1,2]. Self- and co-assembly processes, following principles from synthetic polymers physical chemistry, provide self-organized nanoassemblies using the produced hybrid polymers, detailed physicochemical studies in aqueous media allowing for gathering information on structure and formation routes of the designed nanostructures [3,4]. Such nanoassemblies were evaluated as nanocarriers for drugs or proteins, and also as nanocontainers for water organic/inorganic pollutants. Co-assembly of functionalized polysaccharides with proteins lead to the creation of biofunctional nanoparticulate structures with biomimetic internal morphology. In parallel, hybrid organic-inorganic or organic-biologic nanostructures were formulated by co-assembly of functionalized polysaccharide materials and inorganic nanoparticles with catalytic properties [5,6].

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References

1. Marius-Mihai Zaharia, Florin Bucatariu, Maria Karayianni, Elena-Daniela Lotos, Marcela Mihai; Stergios Pispas. Synthesis of Thermoresponsive Chitosan-graft-Poly(Nisopropylacrylamide) Hybrid Copolymer and Its Complexation with DNA, Polymers, 16, 1315, 2024. https://doi.org/10.3390/polym16101315
2. Stefania Racovita, Mihaela Iuliana Avadanei, Diana-Felicia Loghin, Melinda-Maria Bazarghideanu, Ana-Maria Macsim, Marcela Mihai, Stergios Pispas, Silvia Vasiliu. Smart graft copolymer based on gellan and poly(N-isopropylacrylamide): Synthesis and studies on structure and thermal behavior, Carbohydrate Polymers, 370, 12436915, 2025. https://doi.org/10.1016/j.carbpol.2025.124369
3. Natural–Synthetic Hybrid Nanostructures Formed Through the Interaction of Chitosan with Carboxylate-Ended PNIPAM: Structure and Curcumin Encapsulation, Elena-Daniela Lotos; Maria Karayianni; Ana-Lavinia Vasiliu; Marcela Mihai; Stergios Pispas, Nanomaterials, 15, 350, 2025. https://doi.org/10.3390/nano15050350
4. Maria Karayianni, Elena-Daniela Lotos, Marcela Mihai, Stergios Pispas. Coassembly of a Hybrid Synthetic–Biological Chitosan-g-Poly(N-isopropylacrylamide) Copolymer with DNAs of Different Length, Polymers, 16(21), 3101, 2024. https://doi.org/10.3390/polym16213101
5. Larisa-Maria Petrila, Maria Karayianni, Tudor Vasiliu, Razvan Puf, Marcela Mihai, Stergios Pispas. Stimuli-responsive laccase/chitosan-g-PNIPAM complexes: A sustainable strategy for biodegradation of organic pollutants, International Journal of Biological Macromolecules, 322, 146754, 2025. https://doi.org/10.1016/j.ijbiomac.2025.146754
6. Marcela Mihai, Florin Bucatariu, Daniela Rusu, Marius-Mihai Zaharia, Stergios Pispas. Environmentally friendly in situ synthesis of gold nanoparticles mediated by thermoresponsive Chitosan-g-PNIPAM copolymer, Reactive and Functional Polymers, 2025.

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PL8

Synthesis and application of new adsorptive nanomaterials for environmental protection and human health

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The paper presents the results of scientific research on the synthesis of activated carbons from local renewable raw materials using different physico-chemical methods. As raw materials, walnut shells, peach, apricot, and plum pits, as well as apple wood, were employed. Steam activation procedures were carried out in a rotary reactor and in a fluidized bed. The structural parameters and adsorption capacities of the new porous materials were determined. It was demonstrated that through the activation of charcoal in a fluidized bed, carbon adsorbents can be obtained that comply with the quality standards required by the European Pharmacopoeia Monograph for enterosorbents.

In order to obtain efficient carbon catalysts for the removal of organic and inorganic pollutants from wastewater and natural waters, the activated carbons were oxidized and impregnated with heavy metal ions. For the same purpose, carbon nanomaterials were synthesized via a hydrothermal activation process at high pressure.

The newly developed adsorptive nanomaterials were applied for the purification of wastewater from textile dyeing enterprises, for the potabilization of natural waters, and for the detoxification of the human body.

The paper also presents and describes the portable installation for water potabilization, developed and patented in the Ecological Chemistry Laboratory of the Institute of Chemistry of Moldova State University. The quality of groundwater in different geographical regions of the Republic of Moldova was investigated. The research results demonstrated that only 4–5% of water from artesian and phreatic wells complied with the sanitary standards established by the regulation for "Drinking Water." Technologies for the potabilization of groundwater were developed and implemented in various districts of the Republic of Moldova.

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PL9

Plastics: intercorrelated effects on economics, environment, health

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Nowadays, plastics – materials used in practical all economic sectors (Fig. 1) [1] - are one of the key elements responsible for environment pollution, impacting the future industrial development at global level. Among plastics, synthetic polymers (known as soft materials) alone or in combination with inorganic hard materials (metals, oxides) are responsible for the actually increasing negative impact on the environment. These materials represent a global challenge as their production is increasing every decade (Fig. 2.), while only 9% are recycled, 12 % are incinerated and the rest is thrown away as wastes [2].

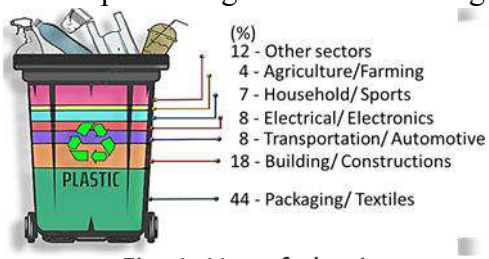

Fig. 1. Use of plastics

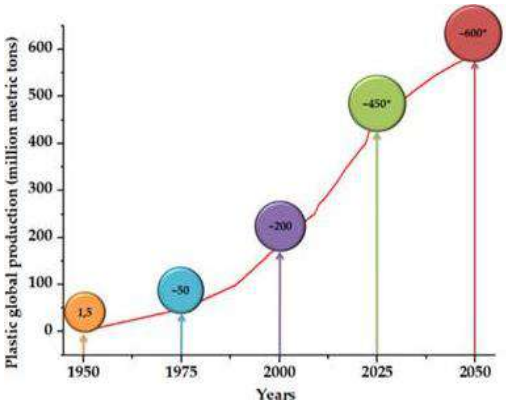

Fig. 2. Evolution of the production

At European and national level, directives and future plans were proposed to ensure the lay of foundation for the development of sustainable, greener plastics through digitalization of their whole life cycle chain and strong involvement of all stakeholders, from academics, industry specialists and consumers to decision makers and politics [3,4].

The work details our view (Fig. 3) meant to accelerate the economy transition toward the targeted climate neutrality foreseen for 2050, by filling the behavioral, technological, demand & supply gaps (negative thinking, lack of engagement, of appropriate technologies and standards for advanced materials, not sufficient expertise and skills, limited demands, inappropriate institutional organization and info sharing). New consumption patterns, more educated consumers, new business models, higher productivity/profitability, more safety in raw material supply, new advanced and more sustainable materials, enabling a cleaner industry and raw materials security are considered methods to achieve this ambitious strategic objective.

Some research results linked to depollution, clean energy production, drug carriers and personalized medicine will be also presented.

References

1. Enache A-C et al. Materials, 2024, 17, 2991.
2. European Environment Agency (EEA)
3. https://eunomia.eco/reports/investigating-options-for-reducing-releases-in-the-aquatic-environment-of-microplastics-emitted-by-products/
4. Planul de acțiune pentru Strategia națională privind economia circulară, Monitorul-Oficial--PI--918Bis--2023.html

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PL10

Self-Purification Processes in Natural Waters: Ecochemical Mechanisms and Environmental Protection Perspectives

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The self-purification of natural waters represents a fundamental ecological process that maintains the chemical balance and biological integrity of aquatic ecosystems. This process encompasses a wide range of interconnected physical, chemical, and biological mechanisms through which pollutants are transformed, immobilized, or degraded. Sedimentation, adsorption, coagulation, oxidation-reduction reactions, photochemical transformations, and microbial biodegradation act synergistically to ensure the natural restoration of water quality. From an ecochemical perspective, self-purification reflects the dynamic equilibrium between pollutant inputs and the self-regulating capacity of aquatic systems.

In recent decades, the understanding of self-purification processes has evolved from empirical observation to quantitative, mechanistic modeling based on biogeochemical principles. Key reactions such as the oxidation of organic matter, nitrification-denitrification, and the formation of reactive oxygen species (ROS) illustrate the coupling between chemical and biological processes within aquatic environments. The role of natural catalysts, including transition metal ions (Fe, Cu, Mn), mineral surfaces, and humic substances, has been recognized as critical in mediating redox transformations and photochemical degradation of organic pollutants.

Current environmental challenges, such as climate change, intensified anthropogenic loading, and emerging contaminants, highlight the importance of assessing the resilience and self-regeneration capacity of water bodies. Increasing temperature, altered hydrological regimes, and nutrient enrichment influence both the kinetics and efficiency of self-purification. Consequently, contemporary ecochemical research integrates field monitoring, laboratory experimentation, and computational modeling to predict the behavior of pollutants and the capacity of ecosystems for natural attenuation.

Advanced analytical methods have enhanced the ability to characterize transformation pathways and identify intermediate products. Meanwhile, microbial ecology provides insights into the composition and function of microbial consortia responsible for degradation and nutrient cycling. Integrating these disciplines supports the development of ecochemically based indicators of water quality and ecosystem health.

The study of chemical self-purification processes of water contributes to the understanding of the mechanisms, control factors and modeling approaches of natural water self-purification. Special attention is paid to the application of ecochemical knowledge in the development of sustainable water management strategies, the design of efficient treatment systems and the restoration of polluted aquatic environments. Important results in this field are possible only through interdisciplinary research and collaboration between chemists, ecologists, hydrologists and environmental engineers, promoting innovative perspectives for environmental protection and sustainable use of aquatic resources in the era of global ecological changes.

Acknowledgments: The results have been obtained in the framework of the project 010603 – Advanced research in computational and ecological chemistry, identification of technological procedures for treatment, formation of water quality and quantity, Institute of Chemistry of the Moldova State University.

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PL11

Aero-semiconductor materials: preparation, properties and prospects for applications

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Three-dimensional aero-semiconductor micro-nano-architectures are an emerging class of highly porous, ultra-lightweight inorganic materials with wide prospects for practical applications. They are similar to aerogels, but are prepared by using technologies different from those derived from a gel.

In this report, aero-semiconductor materials prepared on the basis of ZnO sacrificial templates consisting of 3D architectures built up from interconnected microrods, tetrapods or multipods are reviewed from the point of view of technologies applied for their preparation, properties and applications. The aerographites have been a first subclass of such materials prepared on ZnO sacrificial templates through converting the sacrificial template to graphitic shells in a one-step chemical vapor deposition (CVD) process with toluene or acetylene as carbon source [1]. The advantages of ZnO sacrificial templates are related to abundance of the zinc oxide material, a large variety of technologies available for their fabrication, including those suitable for mass production, and easy methods for removal of the sacrificial substrates during the fabrication of aeromaterials [2].

The technologies applied for the preparation of aero-semiconductor materials include hydride vapor phase epitaxy (HVPE), gold nanodots assisted HVPE with annealing in air, atomic layer deposition (ALD) with subsequent annealing and etching of the sacrificial template, as well as physical vapor transport [3]. It is shown that the introduction of semiconductor components instead of carbonic ones in such technological procedures significantly enlarged the variety of aeromaterials, such as aero-GaN, GaN/ZnO microtubes with nanowires, aero-Ga_2O_3, aero-ZnS, aero-ZnO-ZnS, aero-Ga_2O_3/$ZnGa_2O_4$, and aero-TiO_2.

The characterization of the prepared aero-semiconductor materials is focused on morphological studies by means of scanning electron microscopy and transmission electron microscopy assisted by energy-dispersive x-ray and selected-area electron diffraction pattern analysis, structural and vibration characterization by means of x-ray diffraction and Raman scattering spectroscopy, light emission analysis by means of photoluminescence and cathodoluminescence spectroscopy associated with calculation of color coordinates according to the Commission Internationale de l'eclairage (CIE) 1931 diagram, investigation of electrodynamic properties at the microwave X-band and terahertz frequencies by means of spectral analysis of complex dielectric permittivity, refractive index, and surface impedance, photocatalytic performance investigations under various light illumination conditions, and wetting properties analysis for revealing their hydrophobic/hydrophilic behavior.

The analysis of these properties revealed wide prospects of applications of the developed aero-semiconductor materials in pressure sensing, microfluidics, microrobotics, micro-biological reactors and sensorics, electromagnetic interference shielding at X-band and THz frequencies, photocatalysts for environmental applications, Li-ion batteries, light emission tuned by composition and crystallinity, etc.

References

1. M. Mecklenburg, et al. Adv. Mater. 24 (2012) 3486–3490.
2. Y. K. Mishra, et al. Part. Part. Syst. Charact. 30 (2013) 775–783.
3. V. Ursaki, et al. Beilstein J. Nanotechnol. 15 (2024) 490–499.

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PL12

2D Coordination polymers – a hybrid and more versatile alternative to layered inorganic materials

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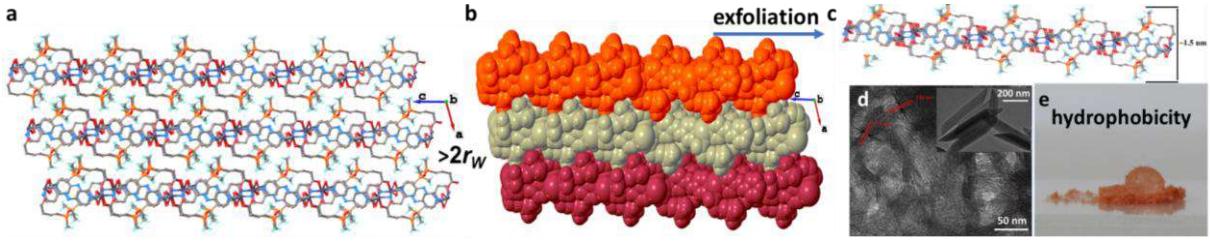
After the discovery of graphene, a monolayer of carbon atoms arranged in a two-dimensional hexagonal lattice, the family of 2D materials has expanded significantly, now including 2D allotropes of various elements, MXenes and others. Due to their remarkable physical properties related to surface, interface and edge effects, these materials are of interest for applications in cutting-edge fields. Two-dimensional coordination polymers (2D CPs) represent an alternative to these inorganic materials. Their hybrid nature allows for structural and application diversity [1]. However, during the crystallization of these compounds, the 2D layers tend to overlap through intermolecular interactions, forming three-dimensional structures that limit the size-dependent properties. The isolation of these thin layers is a challenge that can be solved by top-down (exfoliation of layered aggregates into single or multiple layers with large lateral dimensions) or bottom-up (through structural design and control of crystallization kinetics) methods, each with its limitations. An innovative implementation of the second method could be the use of a permethylated ligand with low surface energy, which favors the formation of 2D structures by anisotropic growth and prevents interlayer interactions, allowing their easy delamination and conferring hydrophobicity (Scheme 1) [2].



Scheme 1. Example of a 2D coordination polymer [L^1L^2Zn], with permethylated ligand L^1 - [OOC-$(CH_2)_3$-$(CH_3)_2Si]_2O$, and coligand L^2 - 4,4′-Azopyridine: a, b - layered packing; c - along-plane view showing the orientation of tetramethyldisiloxane moieties on both sides of the 2D sheet; d - TEM images after exfoliation; e - evidence of hydrophobicity.

Such structures, obtained with bifunctional ligands containing a highly flexible and hydrophobic tetramethyldisiloxane spacer, e.g., 1,3-bis(carboxypropyl)tetramethyldisiloxane or 1,3-bis(cyanopropyl)tetramethyldisiloxane, with or without a coligand, are presented. Several potential applications induced by their particularities (especially organic-inorganic nature and hydrophobicity) have been identified and functional performance evaluated.

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References

1. Dong, R., Pfeffermann, M., Liang, H., Zheng, Z., et al. Angew. Chem. Int. Ed. 54 (2015) 12058.
2. Stoica, A.-C.; Damoc, M.; Zaltariov, et al., React. Funct. Polym. (2021), 168, 105039.

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PL13

Free radicals in health and disease

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Free radicals, including reactive oxygen species (ROS) and reactive nitrogen species (RNS) have long been viewed as harmful by-products of metabolism, yet evidence accumulated over the past decades has revealed their essential role in maintaining physiological functions. At controlled levels, ROS act as key signaling molecules involved in cell proliferation, differentiation, immune defense, and apoptosis. However, when their generation exceeds the buffering capacity of antioxidant systems, oxidative stress develops, leading to cellular and molecular damage.

This work discusses the dual nature of ROS/RNS and the mechanisms through which redox imbalance contributes to the onset and progression of various pathologies. Enzymatic antioxidants such as superoxide dismutase, catalase, and glutathione peroxidase, together with low-molecular-weight antioxidants like vitamins C and E, form an intricate defense network that maintains redox homeostasis. Disturbances in this balance are associated with lipid peroxidation, protein denaturation, enzyme inactivation, and DNA damage – key processes underlying cardiovascular, neurodegenerative, metabolic, and skeletal and other disorders.

Recent findings emphasize that oxidative stress is not merely a damaging factor but also a crucial adaptive signal. Cells possess the ability to sense moderate increases in ROS/RNS and to activate protective pathways, such as upregulation of antioxidant enzymes and repair mechanisms. Understanding where this balance shifts from adaptation to injury remains a major challenge.

Recognizing free radicals as both vital mediators and potential threats opens new perspectives for redox-based therapeutic strategies aimed at restoring physiological equilibrium rather than simply suppressing ROS/RNS formation.

Keywords: reactive oxygen species, reactive nitrogen species, oxidative stress, antioxidants, redox signaling, chronic disease.

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PL14

NMR lipidomics in medicine, molecular sciences and environment

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In terms of number of NMR applications, after chemistry-related topics, metabolomics became a very successful and highly popular NMR topic in the last 30 years. However, although it took a longer time to prove its potential, nowadays NMR lipidomics seems to have an even higher impact in medical research than NMR metabolomics. This fast evolution of the NMR lipidomics was made possible by introduction of carefully developed SOPs, and industry standard solutions for spectra processing, as well as publication of trustful papers demonstrating impressive reproducibility of data, including transferability from various instruments, laboratories and operators into the same statistical model [1-4]. We are applying NMR spectroscopy in metabolomics [5-9] and lipidomics [10-12] for studying complex organisms such as plants [6,10], animals [7], and humans [5,8,9,11,12] with the purpose of advancing scientific knowledge in food sciences [6,10], environment [12], and medicine [5,8,9,11]. We describe here some NMR lipidomics applications in medical diagnosis, food sciences and environmental sciences.

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References

1. S. M. Centelles, H. C. J. Hoefsloot, B. Khakimov, P. Ebrahimi, M. V. Lind, M. Kristensen, N. de Roo, D. M. Jacobs, J. van Duynhoven, C. Cannet, F. Fang, E. Humpfer, H. Schafer, M. Spraul, S. B. Engelsen, A. K. Smilde, Anal. Chem. 2017, 89, 8004–8012.
2. B. Jimenez, E. Holmes, C. Heude, R. F. Marof Tolson, N. Harvey, S. L. Lodge, A. J. Chetwynd, C. Cannet, F. Fang, J. T. M. Pearce, M. R. Lewis, M. R. Viant, J. C. Lindon, M. Spraul, H. Schaefer, J. K. Nicholson, Anal. Chem. 2018, 90, 11962–11971.
3. A. C. Dona, B. Jimenez, H. Schaefer, E. Humpfer, M. Spraul, M. R. Lewis, J. T. Pearce, E. Holmes, J. C. Lindon, J. K. Nicholson, Anal. Chem. 2014, 86, 9887–9894.
4. C. Stavarache, A. Nicolescu, C. Duduianu, G.L. Ailiesei, M. Balan-Porcăraşu, M. Cristea, A.-M. Macsim, O. Popa, C. Stavarache, A. Hîrtopeanu, L. Barbeş, R. Stan, H. Iovu, C. Deleanu, Diagnostics 2022, 12, 559.
5. A. Nicolescu, D. Blanita, C. Boiciuc, V. Hlistun, M. Cristea, D. Rotaru, L. Pinzari, A. Oglinda, A. Stamati, I. Tarcomnicu, A. Tutulan-Cunita, D. Stambouli, S. Gladun, N. Revenco, N. Usurelu, C. Deleanu, Molecules 2020, 25, 5312.
6. M. Balan, A. Nicolescu, C. Stavarache, M. Ciobanu, C. Deleanu, Rev. Roum. Chim. 2013, 57, 175.
7. M. Musteata, A. Nicolescu, G. Solcan, C. Deleanu, Plos One 2013, 8, e81192.
8. T. Andrian, L. Siriteanu, L. Voroneanu, A. Nicolescu, C. Deleanu, Andreea Covic, Adrian Covic, J. Clin. Med., 2024, 13, 5983.
9. C. Deleanu, A. Nicolescu, Biomolecules, 2024, 14, 528.
10. M. Ivanova, A. Hanganu, R. Dumitriu, M. Tociu, G. Ivanov, C. Stavarache, L. Popescu, A. Ghendov-Mosanu, R. Sturza, C. Deleanu, N.-A. Chira, Foods 2022, 11, 1466.
11. L.-A. Stanciulescu, A. Scafa, C. Duduianu, R. Stan, A. Nicolescu, C. Deleanu, M. Dorobantu, Diagnostics 2022, 12, 1675.
12. E. Papadopoulou, A. Nicolescu, L. S. Haug, T. Husøy, C. Deleanu, H. Dirven, B. Lindeman, Environ. Pollution 2022, 308, 119664.

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PL15

Current food system problems and priority research directions in food science

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Food systems are complex networks of value chains with profound effects on human health, environmental sustainability and economic development. They currently face a large number of challenges, some of which are extremely complex: 35% of adults worldwide are overweight/obese, the increasing burden of non-communicable and disabling diseases - diabetes, osteoporosis, anemia, food allergies, amplified by ecological factors. Concerns about the social, environmental and economic sustainability of these systems have become increasingly acute due to challenges such as population growth, urbanization, competition for resources, geopolitical tensions and climate change.

The objective of this review is to present an overview of the existing problems and challenges related to nutrition and food processing in the context of globalized food systems. Given the grand challenges related to Food and Health, the paper aims to highlight the directions of future developments in food science and technology. The research concept underlying a new science is addressed - "Foodomics", defined as "the discipline that studies the food field as a whole with the field of nutrition, applying the same advanced omics technologies to different samples and integrating all the results to have an overall vision that allows improving the health and well-being of the population". The basic tools and main research directions are presented, aimed at ensuring a healthy and sustainable diet: genomics, metabolomics, proteomics, transcriptomics.

Keywords: food systems, foodomics, genomics, metabolomics, proteomics, transcriptomics.

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PL16

From food security to forensic science: stable isotopes (δ^{13}C, δ^{15}N) as tools for reconstructing diet and geographic provenance from human hair

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Stable isotope analysis has become a cornerstone technique for food authentication and security, enabling robust traceability of agricultural products and protection of traditional food heritage. The same isotopic principles that provide unique chemical fingerprints for verifying product provenance can also be applied to human biology, where tissues incorporate dietary and environmental information. This transition, from food traceability to forensic science, illustrates the versatility of isotopic methodologies at the interface of chemistry and medicine.

Human hair is particularly suitable for such applications. Composed primarily of keratin, it is metabolically inert after formation and grows continuously, preserving isotopic signals that reflect an individual's diet and environmental exposure over weeks to months. Carbon (δ^{13}C) isotopic values record the contribution of C3 versus C4 plants in the diet, while nitrogen (δ^{15}N) values provide information on protein sources and trophic level. Together, these markers can be used to reconstruct dietary profiles and to provide partial indications of geographic provenance, complementing traditional forensic methods.

To establish reference data for Eastern Europe, we analyzed scalp hair from 24 Romanian individuals, grouped by age and dietary habits. Isotope ratio mass spectrometry revealed δ^{13}C values ranging between –22.22 ‰ and –18.97 ‰, influenced by the balance of C3 and C4 dietary components. δ^{15}N values differentiated protein intake levels, with mean values of 8.51 ‰ for omnivores, 9.34 ‰ for carnivorous-omnivores, and 7.88 ‰ for vegetarians. Breastfed infants exhibited elevated δ^{15}N values consistent with the trophic-level effect of maternal transfer. Age itself did not significantly influence isotopic variability, confirming diet as the primary factor.

Comparison with international datasets shows that Romanian isotopic signatures are consistent with Eastern European populations. δ^{13}C values allow differentiation from populations on other continents, while δ^{15}N values offer resolution within the same region based on dietary patterns. These baseline data thus provide a valuable framework for future forensic applications.

By bridging its well-established role in food security with emerging applications in forensic science, stable isotope analysis demonstrates its capacity to reconstruct human dietary histories and offer probabilistic insights into geographic background. Human hair, as a temporally resolved isotopic archive, emerges as a promising tool for medico-legal investigations, underscoring the potential of isotopic profiling to support casework in human identification and provenance assessment.

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PL17

Terpene-heterocyclic hybrids as antimicrobial agents

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The increasing incidence of fungal and bacterial infections, along with the rise of antimicrobial resistance, highlights the urgent need for the development of novel molecular entities with improved antimicrobial efficacy. Natural products, and terpenoids in particular, have emerged as a prolific source of bioactive compounds due to their inherent biocompatibility, selective biological activity, and low toxicity profiles. In recent years, the development of hybrid molecules combining terpene structures with heterocyclic scaffolds has gained attention as a promising approach to combat microbial infections, especially those resistant to conventional antibiotics.

In the present study, a series of novel hybrid terpene–heterocyclic compounds incorporating diazine, 1,2,4-triazole, 1,3,4-oxadiazole, 1,3,4-thiadiazole, 1,3-thiazole, 1,3-benzothiazole and 1,3-benzimidazole moieties were synthesized for the first time via multistep synthetic routes starting from commercially available (+)-sclareolide, derived from the labdane-type diterpenoid (-)-sclareol isolated from industrial waste of *Salvia sclarea* L. [1-7].

All synthesized compounds underwent preliminary *in vitro* screening for antifungal and antibacterial activity against pure cultures of fungal strains: *Aspergillus niger*, *Fusarium solani*, *Penicillium chrysogenum*, *Penicillium frequentans*, and *Alternaria alternata*, as well as Gram-positive *Bacillus* spp. and Gram-negative *Pseudomonas aeruginosa* bacterial strains.

Biological evaluation demonstrated moderate to significant antimicrobial activity for several terpene-heterocyclic compounds, indicating their potential as promising therapeutic candidates. Notably, the antimicrobial efficacy of selected compounds has been secured through six patents, further supporting their relevance in drug development.

These promising results highlight the potential of these newly synthesized hybrid molecules as lead candidates for the development of next-generation antimicrobial agents. Moreover, this study contributes to the ongoing advancement of medicinal chemistry and supports the sustainable utilization of renewable natural resources.

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References

1. Kuckova, K.; Aricu, A.; Secara, E.; Barba, A.; Vlad, P.; Ungur, N.; Mangalagiu, I.I. Med. Chem. Res., 2014, 23(3), 1559–1568. https://doi.org/10.1007/s00044-013-0720-3
2. Aricu, A.; Ciocarlan, A.; Lungu, L.; Barba, A.; Shova, S.; Zbancioc, G.; Mangalagiu, I.I.; D'ambrosio, M.; Vornicu, N. Med. Chem. Res., 2016, 25(10), 2316-2323. https://doi.org/10.1007/s00044-016-1665-0
3. Aricu. A.N.; Kuchkova. K.I.; Sekara. E.S.; Barba. A.N.; Dragalin. I.P.; Ungur. N.D.; Melnic, E.; Kravtsov, V.Kh. Chem. Nat. Compd., 2018, 54(3), 455-460. https://doi.org/10.1007/s10600-018-2378-z
4. Blaja, S.; Lungu, L.; Kuchkova, K.; Ciocarlan, A.; Barba, A.; Vornicu, N.; Aricu, A. Chem. Nat. Compd., 2021, 57(1), 101–110. DOI: https://doi.org/10.1007/s10600-021-03292-3
5. Lungu L.; Ciocarlan A.; Smigon C.; Ozer I.; Shova S.; Gutu I.; Vornicu N.; Mangalagiu I.; D'Ambrosio M.; Aricu A. Chem. Heterocycl. Compd., 2020, 56, 578–585. DOI: https://doi.org/10.1007/s10593-020-02703-7
6. Lungu, L.; Cucicova, C.; Blaja, S.; Ciocarlan, A.; Dragalin, I.; Vornicu, N.; Geana, E.; Mangalagiu, I.I.; Aricu, A. Molecules, 2022, 27, 5082-5096. DOI: https://doi.org/10.3390/molecules27165082
7. Lungu, L.; Cucicova, C.; Blaja, S.; Ciocarlan, A.; Dragalin, I.; Barba, A.; Kulciţki, V.; Vornicu, V.; Geana, E.; Mangalagiu, I.I.; Aricu, A. Molecules, 2023, 3(28), 933-946. DOI: https://doi.org/10.3390/molecules28030933

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PL18

Genomics as a driver of health development in Romania and Moldova

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Genomics is becoming a key driver for modernizing Romania's healthcare, enabling earlier diagnosis, more precise therapies and more efficient care pathways. Romania is implementing a national genomics infrastructure through the ROGEN project (Health Programme 2021–2027), while aligning with major EU initiatives such as 1+Million Genomes, the Genomic Data Infrastructure (GDI) and Genome of Europe. In parallel, the European Health Data Space (EHDS) now provides the legal and technical framework to scale secure, interoperable health data use.

Within this ecosystem, ICDG serves as a national capability hub for sequencing, bioinformatics, workforce development and standardization of diagnostic processes. The application of genomics in areas such as rare diseases, oncology, and pharmacogenomics contributes to reducing diagnostic delays, improving therapeutic decisions, and increasing the overall efficiency of the healthcare system. Strengthening infrastructure, expanding professional training, and ensuring interoperability with European standards represent key directions for transforming medical practice in Romania and positioning genomics as a strategic engine of future health development.

Finally, we outline MD–RO collaboration opportunities (cross-border pilots, shared training, and interoperability use cases) that can accelerate safe and equitable implementation of genomic medicine in both countries, leveraging shared standards and the European federation model.

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PL19

Metabolomic research in diagnosis of inborn errors of metabolism

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Introduction. Inborn Errors of Metabolism (IEM) constitute a heterogeneous group of rare disorders resulting from inherited deficiencies of specific enzymes, which disrupt one or more metabolic pathways. Although individually uncommon, IEM collectively occur in approximately 1 in 500 live births. Early diagnosis is essential for initiating appropriate treatment and preventing long-term complications. The aim of this study is to identify and quantify as many metabolites as possible, including those not previously characterized, through both targeted and untargeted analytical approaches.

Materials and methods. For the diagnosis of Inborn Errors of Metabolism (IEM), both targeted metabolomic screening (from dried blood spots, DBS) and untargeted metabolomic profiling (urine NMR spectroscopy) were applied as effective tools for the detection and characterization of IEM in patients from the Republic of Moldova. Complementary analyses, including plasma amino acid profiling and molecular-genetic confirmation, were also conducted.

Results. Through the combined application of targeted and untargeted metabolomic approaches, the following Inborn Errors of Metabolism (IEM) were diagnosed and included in the National Register of Rare Diseases of the Republic of Moldova: Phenylketonuria, Methylmalonic Aciduria, Propionic Acidemia, Glutaric Aciduria, Tyrosinemia Type I, Glycogen Storage Disorders, Galactosemia, Ethylmalonic Aciduria, Mitochondrial Disorders, Urea Cycle Disorders, Non-Ketotic Hyperglycinemia, Biotinidase Deficiency, and others. In addition, a pilot neonatal metabolic screening program using urine NMR spectroscopy was initiated at the Institute of Mother and Child.

Conclusions. Targeted metabolomics enables the quantitative analysis of specific metabolites associated with known metabolic disorders, while untargeted metabolomics offers a comprehensive overview of the metabolic profile, allowing for the identification of unexpected or novel metabolic abnormalities.

Keywords: Inborn Errors of Metabolism, targeted, untargeted metabolomics, rare diseases.

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PL20

NMR metabolomics in plants, animals and humans

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NMR spectroscopy has several, widely accepted, advantages like little requirements for sample preparation, biological fluid's metabolite profile from a single experiment, rapid, nondestructive, reproducible and quantitative, that make it a suitable tool for high-throughput, large-scale metabolomics studies. Measurement of small-molecule metabolites, endogenous or exogenous, provides a chemical "picture" of an organism's metabolic state. Simultaneous characterization of numerous metabolites, or metabolic profiling, is an area of analytical chemistry that uses analytical metabolite measurement with pattern recognition chemometric statistical analysis to characterize complex biochemical mixtures. This technique has wide applicability to a number of fields including medicine, plant sciences, toxicology, and food sciences. For animals and humans, urine and blood serum or plasma are the most commonly used biological fluids for metabolomics-based studies as they both contain hundreds of detectable metabolites and can be obtained non- or minimally invasively. For plant metabolomics, any part of the plant that can be squeezed to obtain some vegetal fluid, can be analyzed. Currently, the 1D nuclear Overhauser enhancement spectroscopy (NOESY) sequence with water suppression is the most commonly used NMR experiment for metabolomics applications, but different other 1D and 2D NMR experiments can be recorded to gain more information about the analyzed biological fluid.

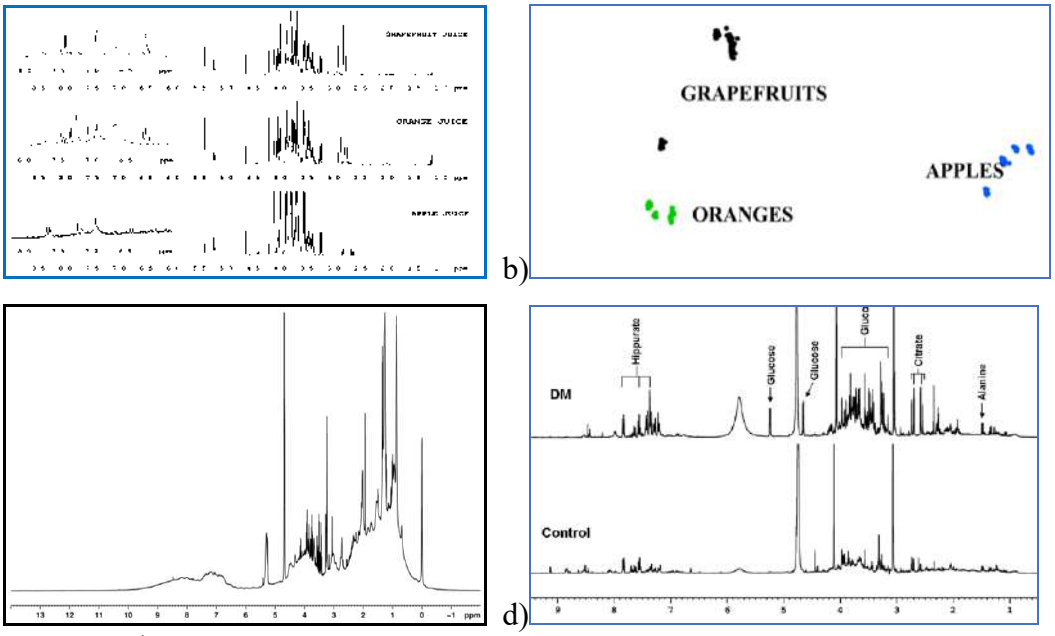

Figure 1. a) ^{1}H NMR spectrum of fresh fruit juices; b) Statistical separation of the juices, based on NMR data; c) ^{1}H NMR spectrum of serum sample; d) ^{1}H NMR spectrum of urine samples.

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KEYNOTE PRESENTATIONS

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KN1

Pyrrol-sulfonamide molecules: small size, vast possibilities

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The majority of nosocomial infections and a considerable share of global mortality continue to be caused by microbial diseases, placing a substantial burden on healthcare systems. This issue is further exacerbated by the growing threat of antimicrobial resistance (AMR), often referred to as a "slow tsunami," with the potential to render current antibiotics ineffective. In light of this, drug discovery efforts are increasingly directed toward the development of novel antimicrobial agents featuring innovative chemical scaffolds and mechanisms of action. Despite the promising activity of single-target agents, clinical experience suggests they are often inadequate in complex biological systems. Consequently, there is a pressing need for the design and development of multi-targeted therapeutic molecules capable of addressing the limitations posed by AMR.

Sulfonamides, some of the earliest antimicrobial agents developed, continue to hold significance in medicinal chemistry due to their wide-ranging biological activities, including antibacterial, antifungal, anti-inflammatory, antioxidant, and anticancer effects. Heterocyclic structures bearing sulfonyl or sulfonamide groups, such as pyrroles, quinazolinones, benzimidazoles, and thiazoles, have demonstrated promising antimicrobial activity, even against multidrug-resistant strains. Pyrrole, in particular, has emerged as a key nitrogen-containing heterocycle, widely utilized not only in pharmaceuticals but also in agrochemicals and advanced materials. Among pyrrole derivatives, pyrrol-2-ones are frequently found in bioactive natural compounds and exhibit various pharmacological properties. Notably, compounds with antioxidant potential are highly valuable, as oxidative damage at sites of inflammation contributes significantly to disease progression; thus, antioxidants help protect cellular structures and maintain tissue integrity.

In this context, two novel series of sulfonamide derivatives featuring a pyrrol-2-one core were synthesized and investigated for their antimicrobial and antioxidant properties. The study focused on the influence of sulfonamide substitution patterns, with 14 different radicals attached at either the *meta* (3-SA series) or *para* (4-SA series) position on the pyrrole ring. Antimicrobial testing against *Escherichia coli*, *Pseudomonas aeruginosa*, and *Candida albicans* revealed that, with few exceptions, compounds in the 3-SA series exhibited superior antibacterial activity compared to those in the 4-SA series. In parallel, antioxidant activity assessed using ABTS and DPPH radical assays showed comparable results between the two series overall; however, several compounds from the 3-SA series demonstrated notably stronger radical scavenging activity, further emphasizing the potential of meta-substituted sulfonamide-pyrrol-2-one frameworks in the design of multifunctional therapeutic agents.

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KN2

Mesoporous chitosan nanofibers: an approach to wound dressings

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Chitosan is a biopolymer extensively studied for integration into biomedical materials due to its advantageous properties, including biocompatibility, biodegradability, and a broad spectrum of bioactivities such as hemostatic, bacteriostatic, and immunomodulatory effects. A further advantage is its versatility in processing, as it can be transformed into films, coatings, hydrogels, nanofibers, or bioprinted constructs, thereby expanding its range of applications. In particular, the processing of chitosan into nanofibers yields biomaterials with characteristics suitable for wound dressings, including morphological similarity to the natural extracellular matrix, high absorbency, semi-permeability, and excellent conformability. Besides, the nanofibers can be prepared by electrospinning, a relatively green and environmentally friendly method. Numerous chitosan-based nanofiber systems have been reported in the literature, demonstrating good performances in animal wound-healing models. However, translation to real-world clinical use remains limited, leaving rooms for further development and optimization.

In this context, the present study proposes a novel approach to the design of wound dressings based on chitosan nanofibers. The concept is centered on idea of bioactive, biodegradable material that eliminates the need for dressing removal, thereby avoiding damage of newly formed tissue, while providing suitable biological activity to promote rapid healing. To achieve this, chitosan nanofibers were prepared using polyethylene oxide with double role, of an electrospinning agent and a sacrificial matrix. This process produced mesoporous fibers with ability to incorporate bioactive agents such as antibiotics, high exudate-retention capacity and enhanced mechanical strength. By loading norfloxacin antibiotic into fibers and reacting at the surface with an antifungal aldehyde, the fibers gained broad antimicrobial activity against Gram-positive and Gram-negative bacteria as well as fungal strains, in vitro cytocompatibility with normal human fibroblasts, and in vivo biocompatibility in rat models. They exhibited rapid swelling and biodegradation in media mimicking wound exudate, and in vivo studies using a rat burn model demonstrated wound closure concurrent with tissue regeneration. All these findings recommend the new nanofiber approach as a platform for developing biodegradable wound dressings [1].

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References

1. Ailincai, D., Cibotaru, S., Anisiei, A., Coman, C. G., Pasca, A. S., Rosca, I., Sandu, A. I., Mititelu-Tartau, L., & Marin, L. (2023). Mesoporous chitosan nanofibers loaded with norfloxacin and coated with phenylboronic acid perform as bioabsorbable active dressings to accelerate the healing of burn wounds. Carbohydrate Polymers, 318, 121135. https://doi.org/10.1016/J.CARBPOL.2023.121135

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KN3

Wearable biosensors for physiological and nutritional monitoring in military contexts: comparative analysis of functionality, monitored parameters, and emerging directions

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Wearable biosensors represent an emerging strategic technology in military health, enabling continuous, non-invasive monitoring of physiological and metabolic parameters under extreme operational conditions. This study conducted a thematic and comparative analysis of 17 scientifically validated biosensors, selected from 26 articles published between 2015–2025, encompassing applications in military personnel as well as sports-analog contexts.

Extracted data covered technical specifications, monitored parameters, transduction principles, usage contexts, and functional scores (portability, accuracy, practical utility) assessed on a standardized scale (1–5). The analysis revealed that 41% of the devices are multimodal, capable of monitoring between 5 and 19 parameters, while the remaining 59% are unifunctional. The most frequently monitored variables included heart rate (HR, 82% of biosensors), heart rate variability (HRV), oxygen saturation (SpO_2), respiratory rate, and body temperature—highlighting a primary focus on cardiovascular and respiratory functions. Metabolic parameters (glucose, lactate, salivary biomarkers) remain poorly integrated, indicating an underexploited potential for development.

From a technological standpoint, electrophysiological (35%) and optical (24%) biosensors dominate due to their portability and sensitivity in field conditions. The majority of included studies originated in the United States (62%), followed by Australia, Portugal, China, Greece, and New Zealand. Testing contexts varied: 38% in real missions, 35% in simulated training, and 27% in laboratory settings, underscoring the current trend toward ecological validation.

Functional scoring indicated high averages for portability (4.52) and practical utility (4.68), moderate accuracy (4.16), and an overall mean total score of 13.36 out of 15—demonstrating good adaptability to field conditions. However, challenges related to energy autonomy, robustness under extreme conditions, and multi-parametric integration remain significant barriers to large-scale operational deployment.

The analysis identifies three priority directions for innovation: (1) integration of multisensor architectures capable of simultaneously tracking cardiovascular, respiratory, metabolic, and physiological stress parameters; (2) development of energy-autonomous systems using kinetic or thermal energy harvesting; and (3) improved robustness and accuracy under severe operational stressors. Expanding the range of real-time nutritional biomarkers monitored (glucose, lactate, cytokines, oxidative stress markers) is essential for comprehensive physiological assessment in mission-critical environments.

References

1. Țurcanu, D., Siminiuc, R. Software for Nutritional Assessment of People with Gluten-Related Disorders. J. Eng. Sci. 30, 164–172 (2023). https://doi.org/10.52326/jes.utm.2023.30(3).12
2. Siminiuc Rodica, Dinu Țurcanu. Wearable Biosensors for Nutritional Monitoring of Soldiers: The Future of Prevention in Operational Theaters. ICNBME 2025. IFMBE Proceedings, vol. Springer, Cham.

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KN4

Romanian experience of Tolvaptan treatment in patients with rapid progressive ADPKD

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Background and objective. Autosomal dominant polycystic kidney disease (ADPKD) progresses with a steady decline in kidney function. Tolvaptan is the only approved therapy that slows progression, but real-world data remains limited. In this paper we assessed the tolerability, safety, and implementation barriers of Tolvaptan treatment in a tertiary center in Romania.

Methods. A retrospective, observational, single-center study was performed at the Dr. C.I. Parhon Clinical Hospital, Iasi, from February 2022 to August 2025. We reviewed records of adult patients (≥18 years) with ADPKD and rapid progression (classified as Mayo 1C–1E). The patients were monitored monthly over 18 months, with quarterly clinical assessments for: blood pressure, weight, urine output; kidney function, electrolytes, cytolysis enzymes, INR, bilirubin, uric acid. Primary outcome: tolerability (withdrawals and other reasons). Secondary outcomes: hepatic and aquaretic events, dosing/titration patterns, and distribution of events by gender and age group.

Results. Out of the 124 eligible participants, 112 ADPKD patients initiated Tolvaptan and only 12 did not start the treatment (due to reluctance regarding adverse effects). The baseline characteristics: 59.8% of the patients were female; 65% had hypertension and 7.1% diabetes; the CKD stages: 28% G1, 40% G3; Mayo classes:1D 33%, 1E 14%.

In term of the primary outcome, by August 2025, 93 remained on therapy and 19 (17%) discontinued. The mean time on therapy was 16 months for continuers *vs.* 3 months for discontinuers. For the discontinuers: 8/19 (42%) withdrawn for treatment-related reasons, predominantly polyuria–polydipsia, headache/fatigue, and GI intolerance and 11/19 (58%) for non-medical reasons, such as access/insurance issues or loss to follow-up.

In term of the secondary outcomes: all patients started with a dose of 45/15 mg and after 1 year (evaluable N=44), 81.8% were at the dose of 60/30 mg. Hepatic events (ALT/AST elevations) occurred in ~33.9%, with only 2 patients that exceeded 3× the upper limit of normal, most with concomitant hepatotoxic factors, and therapy was generally resumed after enzyme normalization.

Mean diuresis on therapy was ~5.8 L/day; polyuria led to discontinuation in 5 patients and limited up-titration in others. Discontinuations were balanced by gender.

Conclusions. In our real-clinic experience, Tolvaptan is a feasible treatment for patients with rapid progressive ADPKD, but tolerability is constrained by aquaretic effects and mostly mild–moderate hepatic cytolysis. These findings support standardized counseling, stringent hepatic monitoring, and adherence-support strategies to translate trial efficacy into routine clinical care.

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KN6

NMR spectroscopy as a tool in checking dairy foods for conformity: detecting the addition of oils and fats of non-dairy origin

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The substitution of milk fat with lower-cost oils or fats is among the most common fraudulent practices in the dairy industry, due to the high value of milk fat in the production of dairy derivatives. The main adulterants include vegetable oils (such as soybean, sunflower, coconut, and palm oil) and animal fats (such as beef tallow and pork lard) [1-2]. The structural diversity of triacylglycerols is reflected in specific resonances within the NMR spectra of fats and oils.

In this work, we propose a novel approach based on three NMR descriptors associated with chain length, the presence of butyric and/or linolenic acid moieties, and the degree of unsaturation, to characterize fat samples. A 3D representation of these descriptors enables the clustering of samples according to fat type. Further development of the method-including data processing and geometrical characterization of the clusters-facilitates the detection of non-dairy fats in cheese.

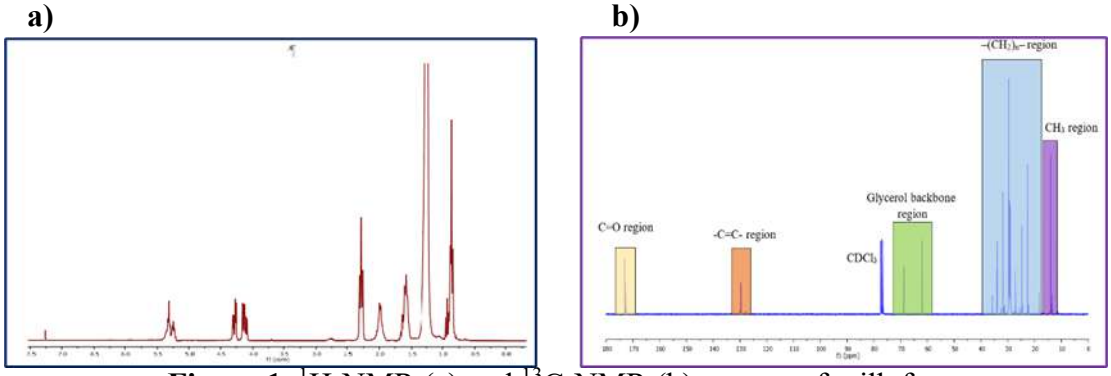

Figure 1. ^{1}H-NMR (a) and ^{13}C-NMR (b) spectra of milk fat.

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References

1. Hanganu, A., Chira, N.A., 2021. When detection of dairy food fraud fails: An alternative approach through proton nuclear magnetic resonance spectroscopy. J. Dairy Sci., 104(8):8454–8466.
2. Pereira, C.G., Leite, A.I.N., Andrade, J., Bell, M.J.V., Anjos, V., Nunes Leite, C.A.I., Andrade, J., Bell, M.J.V., Anjos. V., 2019. Evaluation of butter oil adulteration with soybean oil by FT-MIR and FT-NIR spectroscopies and multivariate analyses. Lebensm. Wiss. Technol., 107:1–8. https://doi.org/10.1016/j.lwt.2019.02.072.

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KN7

Optimized *Porphyridium purpureum* biomass as a source of reducing sugars for AgNPs biosynthesis

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Porphyridium purpureum is a marine microalga of significant biotechnological interest, known for producing valuable bioactive compounds, particularly polysaccharides with regenerative, antioxidant, and antiviral properties [1]. Due to their biocompatibility and biodegradability, these polysaccharides find applications in the food, nutraceutical, and pharmaceutical industries [2,3] and also serve as excellent supports for the synthesis of metallic nanoparticles, providing a rich source of functional groups [4]. Our study focused on optimizing culture conditions to enhance the yield of natural biopolymers in *Porphyridium purpureum* biomass, isolating the reducing sugar fractions, and employing them for silver nanoparticle biosynthesis. The *Porphyridium purpureum,* strain CNMN-AR-01 was cultivated in Brody mineral medium supplemented with 1 mL/L amyl alcohol. Biomass harvested at the end of the 14-day cultivation cycle displayed a complex bioactive profile suitable for advanced biotechnological applications, with increases of and 29% in reducing sugars compared to the control. The reducing sugar fraction was obtained through advanced extraction and separation techniques from *Porphyridium purpureum* biomass enriched with these biopolymers, and used for silver nanoparticles synthesis. $AgNO_3$ was added to the reducing sugar fraction at a ratio of 10 mg per 1 mL of reducing sugar solution. The mixture was incubated at room temperature under constant stirring for 120 minutes, during which the reducing sugars facilitated the conversion of silver ions (Ag^+) into metallic nanoparticles (Ag^o). FTIR analysis confirmed the presence of hydroxyl, carbonyl, and amine groups involved in the colloidal stabilization of the nanoparticles. The result is a stable bioactive system with promising applications in biotechnology and biomedical fields.

Acknowledgements: This research was carried out within the framework of the bilateral complex project 25.80013.8007.12ROMD.

References

1. Li, T. et al. Growth and Biochemical Composition of Porphyridium purpureum SCS-02 under Different Nitrogen Concentrations. *Mar. Drugs,* 2019, *17,* 124. https://doi.org/10.3390/md17020124
2. Cáceres-Ferroni, F. et al. Effect of culture medium composition and reuse on the growth of *Porphyridium cruentum*. New Biotechnology, 2025, 90, 65-76. https://doi.org/10.1016/j.nbt.2025.09.001
3. Bayu, A. et al. Biological and technical aspects on valorization of red microalgae genera *Porphyridium.* Biomass Conv. Bioref, 2023, 13, 12395-12411. https://doi.org/10.1007/s13399-021-02167-5
4. Wang, C. et al. Preparation, Characterization and Application of Polysaccharide-Based Metallic Nanoparticles: A Review. Polymers, *2017, 9, 6*89. https://doi.org/10.3390/polym9120689

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KN8

Soil microorganisms as indicators of soil pollution by POPs

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Soil pollution with harmful and persistent substances remains one of the most pressing environmental challenges in the Republic of Moldova, particularly near former pesticide storage facilities. Nationwide, at least 1,600 sites are contaminated with persistent organic pollutants (POPs), compounds that not only degrade soil quality but also endanger natural ecosystems and pose risks to the health of plants, animals, and humans. Addressing this issue requires, among other things, reliable indicators to assess and monitor the toxic impact of POPs and to evaluate the success of soil remediation measures.

Soil microorganisms are widely regarded as promising indicators of environmental stress. Their activity reflects the state of the soil environment, as it depends on the quantity and quality of soil organic matter, the availability of nutrients, and the influence of various environmental factors. Soil microbial biomass (SMB) is among the most frequently used microbiological indicators. Because POPs significantly affect microbial activity, changes in SMB can serve as a potential measure of soil pollution. However, the efficiency of this indicator is limited, as SMB is also subject to strong seasonal dynamics and can be influenced by microbial adaptation, including the ability to partially degrade POPs. Consequently, the interpretation of SMB changes in polluted soils requires careful consideration of multiple confounding factors.

The aim of our study was to estimate the sensitivity of SMB to long-term contamination by POPs (DDTs and HCHs) in typical chernozem soils of Moldova and to explore possible ways of improving the diagnostic value of microbiological indicators. Soil samples were collected from three sites near a former USSR pesticide storage facility in the Sangerei district. The sites represented three levels of contamination: negligible (below maximum allowable concentrations [MACs]), medium (2–3 times above MACs), and high (≥10 times above MACs). In addition, unpolluted soil from a nearby forest shelterbelt was used as a control. SMB was repeatedly determined during three contrasting seasons.

Our results showed that SMB was more strongly influenced by the organic matter content of the soil than by POP concentrations. The relative differences in SMB between control and contaminated soils also varied markedly with season. In many cases, seasonal fluctuations in SMB within both polluted and unpolluted soils exceeded the differences between them at any given time. These findings confirm that absolute or relative SMB values alone are insufficient for reliable assessments of POP pollution.

Our findings suggest that a more promising strategy involves studying the functional capacity of soil microorganisms, particularly their role in organic matter mineralization and other key ecological processes. Such functional indicators may overcome the limitations of SMB measurements and provide more robust tools for evaluating the impact of POPs and the effectiveness of soil remediation measures.

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KN9

Dietary patterns in Eastern Europe (2010–2022): comparative FAOSTAT analysis and implications for non-communicable disease prevention

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Eastern European countries are experiencing rapid dietary transitions that may influence the risk profile for non-communicable diseases (NCDs). Multi-country, long-term comparisons with detailed resolution by major and subgroups of foods are limited, yet such analyses are essential to understanding the nutritional determinants of NCD burden. This study maps dietary patterns across Eastern Europe from 2010–2022, evaluates their associations with macronutrient/fiber intake and obesity prevalence, and discusses their implications for NCD prevention strategies.

FAOSTAT Food Balance Sheet (FBS) data were analyzed for 10 countries. Multi-year averages (2010–2022) of per capita daily energy availability (kcal) were calculated for nine major food groups and selected subgroups (cereals, meats, vegetable oils). Data were standardized (Z-scores) to enable cross-country comparisons. Principal trends in dietary composition were identified, and nutrient profiles (macronutrients, fiber, total energy) were benchmarked against EFSA recommendations. Associations with national obesity/overweight prevalence (2010–2022 averages, official sources) were assessed using Pearson and Spearman correlations (α=0.05). Data processing involved Excel and Power Query; visualization was performed in GraphPad Prism, with optional clustering analyses in PAST.

Across the region, diets are dominated by "Cereals, excl. beer" and "Animal products," with notable variation in "Starchy roots" and "Animal fats." Subgroup patterns reveal distinct national profiles—maize dominance in Romania and Bulgaria, barley/rye in Belarus and Poland, sunflower oil prevalence in Ukraine, Moldova, and Bulgaria, and rapeseed oil in Czechia and Poland. Overall, carbohydrate energy shares (%E) meet EFSA ranges, while fat energy shares (%E) exceed the recommended levels. Fiber intake remains below optimal in most cases. Correlations between national dietary trends and obesity prevalence were largely non-significant, reflecting the ecological scope of the data and the influence of unmeasured factors (physical activity, lifestyle, food environments).

The 2010–2022 comparative dietary landscape offers a valuable baseline for public health action. Diets high in saturated fats and low in fiber contribute to metabolic risk factors underlying cardiovascular diseases, type 2 diabetes, and certain cancers. By combining population-level dietary surveillance with targeted nutrition interventions, countries can address dietary risk factors within NCD prevention frameworks. Regional cooperation could enable harmonized dietary guidelines, culturally adapted education campaigns, and monitoring systems aligned with WHO's NCD Global Action Plan targets.

This study provides an evidence-based comparative assessment of Eastern European dietary patterns and their potential contribution to NCD risk. It underscores the importance of sustained dietary monitoring and coordinated regional strategies to reduce the burden of non-communicable diseases.

References

1. Siminiuc, R.; Țurcanu, D.; Siminiuc, S.; Vîrlan, A. Integration of Nutritional and Sustainability Metrics in Food Security Assessment: A Scoping Review. Sustainability, 17, 2804, 2025. https://doi.org/10.3390/su17072804

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KN10

Bridging the gap between cancer research and clinical care with nanomedicine

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Nanomedicine, resulting from the integration of nanotechnology with medicine, holds potential in bridging the gap between cancer research and clinical care, offering innovative solutions for early/precise diagnosis, targeted therapy, and monitoring. This is based on the fact that recent advancements in nanostructured drug delivery systems have enhanced therapeutic efficacy while minimizing side effects [1]. Using nanoparticles as contrast agents can improve the diagnostics while reducing the time of investigation, for instance in MRI. Furthermore, nanotechnology enables the integration of diagnostic and therapeutic modalities, creating theranostic platforms for personalized cancer care [2]. All these statements are validated by products of nanomedicine approved by FDA and EMA for use in clinical settings and on the pharmaceutical market (e.g, Doxil, Onivyde, Abraxane, Lipodox, Vyxeos, NanoTherm, Feridex) [3], reinforcing the capacity of nanomedicine to address real-world challenges, such as cancer. Based on this real potential of nanomedicine, a field still requiring extensive preclinical research but already revolutionizing the medical paradigm, the Regional Institute of Oncology in Iași, Romania, has made significant steps in research and innovation by adopting nanomedicine in its scientific agenda and establishing a nanomedicine-oriented research laboratory. Therefore, Since January 2021, IRO initiated the setting up of the Nanotechnology Laboratory (NTL) through a H2020-ERA Chairs initiative. Although the NTL is a relatively new facility, its team is committed to contributing to global cancer research efforts and advancing the application of nanomedicine for both diagnostic and therapeutic purposes [4]. At NTL, research is centered on three key areas: (i) development of inorganic nanoparticles for drug delivery and imaging, (ii) development of microemulsions and multifunctional liposomes for targeted drug delivery, and (iii) the creation of early cancer detection methods using combined Surface Enhanced Raman Spectroscopy (SERS) and Multivariate Analysis (MVA) of vibrational spectra obtained from various biological fluids. Central to these efforts is the rational design of nanoparticles tailored to meet specific therapeutic or diagnostic objectives. To date, our team has successfully developed: (i) magnetic nanoparticles and layered double hydroxides with diverse functionalities, (ii) microemulsions and liposomes with varying compositions to better understand the role of formulation in drug loading, retention, and controlled release, and (iii) plasmonic nanoparticles of varying shapes and sizes, which serve as the foundation for new solid substrates that enhance the Raman signal specific to biofluids.

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References

1. Ai Z., et al., Int. J. Pharmaceutics: X, 9 (2025) 100314;
2. Sergeeva O.V., et al., Front. Bioeng. Biotechnol., 12 (2025) 1499474;
3. Halwani, A.A., Pharmaceutics, 14 (2022), 106;
4. Wang B., et al., Signal Transduction and Targeted Therapy, 9 (2024) 200.

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KN12

Fusion of art, science and education: Kabuki phenotype

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The "Kabuki phenotype" describes the distinct set of physical, developmental, and behavioral features that characterize individuals with Kabuki syndrome. International consensus on the diagnostic criteria for Kabuki syndrome was established in 2019. The criteria typically involve meeting specific requirements for developmental delay/intellectual disability and characteristic facial features, with genetic testing serving as the most definitive tool.

Kabuki syndrome (KS; also known as Kabuki make-up syndrome and Niikawa-Kuroki syndrome) is a rare inherited genetic syndrome with a heterogeneous phenotype and affects multiple organ systems: specific facial characteristics, intellectual disability, skeletal anomalies, and potential heart, kidney, endocrinologic and immune system issues. A broad and continuous spectrum of clinical phenotypes is associated with KS, with notable variability between affected individuals. KS derives its name from the distinct dysmorphic facial features resembling traditional Japanese 'Kabuki' theatre actors.

The pathogenesis of Kabuki syndrome is defined by epigenetic modifications during embryogenesis that regulate the expression level of genes (*KMT2D* and *KDM6A*) by the on and off switch of chromatin. Individuals with a *Kabuki-like syndrome* may have mutations in other genes that affect similar pathways, such as chromatin remodeling and transcriptional regulation.

Differential diagnosis includes CHARGE, 3MC, Hardikar syndromes, *KAT6B*-related disorders, and other genetic disorders involving chromatin regulation.

Increased awareness and understanding of KS among clinicians is important for diagnosis, management and for primary care of patients. Kabuki syndrome occurs spontaneously, very rarely inherited, autosomal dominant and X-linked.

Care for KS patients includes the control of physical and psychomotor development during childhood, rehabilitation and multi-specialist care.

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KN13

A clinical study involving serum irisin assays in post-menopause: blood markers correlates (project IRI-OP-OB)

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Background. Irisin represents a recently detected hormone that only during latest years has been studied at clinical levels. So far, it seems to play an important role in relationship with the glucose profile, body fat content, and bone metabolism. Cutting edge researches have been placed irisin among the pathogenic loops of various ailments, including diabetes.

Objective. To analyze the levels of circulating irisin with regard to the mineral metabolism and glucose status assessments.

Patients and methods. This clinical, prospective, international study included females in menopause who were aged between 50 and 80 years. Subjects prior diagnosed with any bone metabolic disease, oncologic conditions or those who were previously under anti-osteoporotic or insulin therapy was excluded. Ethical Boards approval included: 32/30.09.2024 (Bucharest), 97/20.11.2024 (Chisinau). Fasting irisin was tested based on ELISA (MyBioSource) in ng/mL Statistical significance cut-off was considered at p-value <0.05.

Results. 74 patients were included with a mean age of 62.55 ± 9.26 years (median of 62). Serum irisin was of 62.21 (mean), respectively, 76.54 (median) ng/mL. Irisin statistically significant correlated with serum fasting insulin (median of 6.47 µUI/mL; ranges: 1.3 to 33.01) with a correlation coefficient of 0.402 (p = 0.0035). Also, glycated hemoglobin A1c (median of 5.7 %) correlated with fasting irisin (r = 0.246, p = 0.036). Body mass index (average value of 30.79 ± 5.79) statistically significant correlated with irisin (r = 0.37, p = 0.0004). When it comes to the bone turnover markers, the correlations did not reach the p-value cut-off of 0.05: bone resorption marker CrossLaps, bone formations markers P1NP, alkaline phosphase, osteocalcin. Irisin does not seem to be correlated with the patients' age (r = 0.07, p = 0.48).

Conclusion. According to the results that have been achieved at this point in the current research (which is undergoing), circulating irisin assays might prove a good correlation profile with the glucose status as reflected by the insulin and glycated hemoglobin A1c, while the essence of the blood mineral metabolism and bone turnover markers might not be captured by testing irisin, potentially related to bone cells receptors activity involvement or with interferences at bone mineral density, rather than serum markers.

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KN14

Diagnostic and therapeutic management of colonic papillomatosis associated with pediatric ulcerative colitis

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Introduction. Colon papillomas in children are known as benign, non-cancerous growths and represent the most common type of colon polyps. Pediatric ulcerative colitis is an inflammatory bowel disease that may occur independently or in association with colon papillomas, often presenting with rectal bleeding. Some children with ulcerative colitis may also develop post-inflammatory colon papillomas or polyps as a rare complication, which can be misinterpreted as colon cancer.

Purpose of the study. To present the challenges in the diagnostic and therapeutic management of colon papillomatosis associated with ulcerative colitis, primarily diagnosed in a 17-year-old adolescent with a partial therapeutic response.

Materials and methods. The study is based on data collected from the inpatient medical records of a patient hospitalized as an emergency case due to rectal bleeding, with written consent obtained from the family. The diagnosis was established via diagnostic rectoscopy and endoscopic removal of colon papillomas, followed by hemostasis and histological examination of the formations. The diagnosis was reconfirmed through colonoscopy during relapse episodes with recurrent rectal bleeding and appearance of new colon papillomas. The severity of the intestinal inflammatory process was assessed using the PUCAI score, along with the presence of intestinal inflammatory markers (elevated erythrocyte sedimentation rate, leukocytosis, C-reactive protein, and calprotectin), microbiological investigations, and comprehensive multidisciplinary evaluations for differential diagnosis, in accordance with the guidelines of the European Society for Paediatric Gastroenterology, Hepatology and Nutrition (ESPGHAN). The patient was monitored by a multidisciplinary team including pediatricians, gastroenterologists, surgeons, a psychologist, a pulmonologist, and a gynecologist.

Results and discussion. The female patient initially presented as an emergency case with abdominal pain, repeated rectal bleeding, diarrhea (<12 stools in 24 hours), and low-grade fever. She had been symptomatic for the past six months, with reported weight loss of 6 kg, following an episode of acute enteroviral infection. Her maternal grandfather died from gastrointestinal cancer, while both parents are considered healthy. At age 15, the adolescent received the HPV vaccine. Clinical and paraclinical evaluation revealed an age-appropriate physical condition, clinical signs typical of ulcerative colitis with rectal bleeding, dehydration, and metabolic acidosis, PUCAI score of 65, grade II anemia, elevated fecal calprotectin and CRP, presence of *Clostridium difficile* (toxins A and B), and *Klebsiella pneumoniae* in stool, with no evidence of acute epidemic intestinal infections. Celiac disease and specific tuberculosis infection were excluded. Treatment was initiated with supportive therapy, including mesalazine, metronidazole, vancomycin, intestinal and later systemic corticosteroids, and humanized monoclonal IgG1κ antibodies, which the patient continues to receive. After seven months of biological treatment, partial improvement was achieved, with reduced disease severity, though episodes of relapse and hemocolitis persisted.

Conclusions. This is the first reported case of colon papillomatosis associated with ulcerative colitis diagnosed in a 17-year-old adolescent, showing a fluctuating and refractory course despite complex therapy. The correlation between intestinal papillomatosis and ulcerative colitis activity requires further multidisciplinary research.

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KN15

Robotic surgery in hepato-bilio-pancreatic tumor pathology: indications, advantages and future perspectives in research field

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Robotic surgery offers increased precision, reduced blood loss, minimal postoperative pain, and faster recovery. It allows for minimally invasive operations, facilitates complex reconstructions (such as biliary-digestive anastomoses) and ensures a safer excision of tumors with better visualization and preservation of healthy tissue. This leads to lower risk of complications and a more rapid reintegration of the patient into daily life compared to traditional or laparoscopic techniques.

This approach is recommended in both benign and malignant hepato-bilio-pancreatic tumor conditions (liver, bile ducts, pancreas), especially when minimally invasive approaches are indicated. Robotic surgery is highly useful in cases requiring preservation of organ function and precise excision, and it is indicated for complex surgeries where the limit of conventional laparoscopy is surpassed.

The author underlines all the informations above by exemplifying with his experience in robotic surgery.

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KN16

Treatment of upper digestive bleeding in surgical patients

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Upper digestive bleeding is a severe complication in surgical patients, that rises their morbidity and mortality rates.

This complication can be classified as early or late, depending on the postoperative moment it occurs.

The treatment of upper digestive bleeding in these patients can be conservative, endoscopic or surgical.

Considering the fact that the surgical patient is a fragile patient, with high operative risk, it is preferable in these cases to avoid the reintervention. The choice of endoscopic timing is also very important: the patient must be in a stable state, because endoscopy is also an invasive procedure.

The endoscopic treatment of the surgical patient has some characteristics, because it is vital to protect the integrity of the anastomosis (if the surgery involved the superior digestive tract), and the endoscopic technique must be adapted consistently. Therefore, it is important to use a flexible endoscope, to insufflate minimally and to utilize hemostatic techniques that do not compromise the anastomotic integrity.

The hemostatic techniques are the same used in general in case of upper digestive bleeding, and we want to remind that injecting adrenaline alone is not a sufficient hemostatic technique. There are also new methods that we want to discuss, like OVESCO, Hemospray or Purastat, methods that can be used when the classic techniques did not work.

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KN18

Deep eutectic solvents – a green route in composite materials

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Deep Eutectic Solvents (DES) are a new generation of solvents comprising mixtures of cheap and readily available components which generate eutectics with melting points significantly lower that of their individual components due to ion–dipole interaction or hydrogen bonding. They are ionic green solvents which are not volatile, not flammable and a low-cost alternative to other organic solvents. Their unique properties recommend them in varied practical applications ranging from extraction and biocatalysis to biomedical ones. In biomedical field NADES can be used as biopolymer modifiers, acting as template delivery compounds also knows as "therapeutic deep eutectic solvents", being able to solubilize and stabilize different pharmaceutical products [1]. NADES are interesting liquid-like gels in which H-bonds mediate anion binding, and are able to produce major changes in bulk material characteristics. They are developed as a good alternative for poor soluble drugs, being used as excipients in the pharmaceutical industry [2]. Interest in NADES for composite materials useful for pharmaceutical applications is recent. They possess intrinsic antimicrobial activity, can promote absorption and diminish phenomena like polymorphism or degradation [3]. Although there is a wide range of materials based on natural and synthetic polymers, here we report the utilization of DES in multicomponent matrices intended for application in corneal repair.

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References

1. Marques Silva, J.M.; Reis, R.L.; Paiva, A.; Duarte, A.R.C. Design of functional therapeutic deep eutectic solvents based on choline chloride and ascorbic acid. ACS Sustain. Chem. Eng. 6 (2018) 10355–10363.
2. Lomba, L.; García, C.B.; Ribate, M.P.; Giner, B.; Zuriaga, E. Applications of Deep Eutectic Solvents Related to Health,Synthesis, and Extraction of Natural Based Chemicals. Appl. Sci. 11 (2021) 10156.
3. Filip, D.; Macocinschi, D.; Balan-Porcarasu, M.; Varganici, C.-D.; Dumitriu, R.P.; Peptanariu, D.; Tuchilus, C.G.; Zaltariov, M.-F. Biocompatible Self-Assembled Hydrogen-Bonded Gels Based on Natural Deep Eutectic Solvents and Hydroxypropyl Cellulose with Strong Antimicrobial Activity, Gels, 8(10) (2022) 666.

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KN19

Optimization of anionic surfactant removal using gallic acid-assisted Fenton oxidation

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Water pollution caused by anionic surfactants, such as sodium dodecylbenzenesulfonate (SDBS), remains a significant environmental issue due to their persistence in aquatic environments and their toxicity to aquatic life. Traditional wastewater treatment technologies are often inadequate for fully degrading these compounds, which has prompted growing interest in Advanced Oxidation Processes (AOPs). These processes rely on the generation of hydroxyl radicals (HO•), highly reactive and non-selective species capable of oxidizing a broad range of organic pollutants due to their high oxidation potential ($E° \approx 2.8$ V).

This study explores the influence of gallic acid (GA) on the efficiency of Fenton-based AOPs in degrading SDBS. Experiments were conducted to monitor the degradation of SDBS both in the absence and presence of GA under varying reaction conditions. The oxidation process was tracked by measuring the residual concentration of SDBS spectrophotometrically at 650–660 nm, using a methylene blue extraction method. Three experimental variables were evaluated: the pH of the reaction medium (3.0, 5.0, 7.3, and 8.0), the concentration of gallic acid (25, 30, and 35 mg/L), and the amount of Fe^{2+} ions, with the initial SDBS concentration maintained at 20 mg/L across all trials.

The findings indicate that gallic acid enhances the degradation of SDBS when applied at appropriate concentrations. The most effective removal occurred at a GA concentration of 30 mg/L, where degradation reached 90–94% within the first 10 minutes, suggesting robust HO• radical generation and high system activity. Gallic acid was found to facilitate the regeneration of Fe^{2+} by forming soluble complexes with Fe^{3+}, thereby sustaining the redox cycle and increasing hydroxyl radical production. At lower GA concentrations (<25 mg/L), the process was slower, likely due to insufficient reductant availability. In contrast, higher GA concentrations (>35 mg/L) appeared to hinder the reaction, possibly due to competitive scavenging of HO• radicals by excess gallic acid.

These results demonstrate that gallic acid can act as an efficient promoter of Fenton-based AOPs for surfactant degradation, provided that its concentration is carefully controlled to avoid inhibitory effects.

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References

1. Tarafdar, A., & Sinha, S. (2018). "A sensitive spectrophotometric method for the estimation of anionic surfactants using methylene blue." Analytical Chemistry Letters, 8(5), 639–650.

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KN20

Design and synthesis of new (pyrrolo)indolizine derivatives as potential anticancer agents

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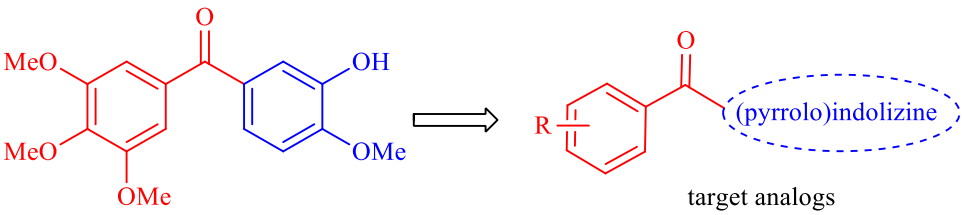
Fused heterocyclic structures such as indolizines have garnered considerable interest in pharmaceutical chemistry due to their presence in compounds exhibiting a wide range of biological activities [1-3]. Notably, certain indolizine derivatives designed as Phenstatin analogs have demonstrated anticancer properties, including the inhibition of tubulin polymerization. Building on our group's established contributions to this area, we have extended our research to (pyrrolo)indolizines, recognizing their potential as scaffolds for the development of novel therapeutic agents [3].



Phenstatin target analogs

This study presents the design and synthesis of novel (pyrrolo)indolizine derivatives, with a focus on exploring diverse substitution patterns on the molecular scaffold. A key step in the synthetic strategy involved a [3+2] cycloaddition reaction to construct the fused heterocyclic core. A series of (pyrrolo)indolizine compounds was successfully synthesized and subsequently evaluated for their anticancer potential and the results are discussed herein.

Aknowledgments
We acknowledge the CERNESIM Research Centre at Alexandru Ioan Cuza University of Iasi for the NMR experiments.

References

1. Ramalakshmi N., Amuthalakshmi S., Yamuna R., Smith A., Arunkumar S., Der. Pharma. Chem. 13(2), 60-69 (2021).
2. Sardaru M.C., Craciun A.M., Al Matarneh C.M., Sandu I.A., Amarandi R.M., Popovici L., Ciobanu C.I., Peptanariu D., Pinteala M., Mangalagiu I., Danac R., J. Enz. Inhib. Med. Chem. 35(1), 1581-1595 (2020).
3. Amariucai-Mantu D., Antoci V., Sardaru M.C., Al Matarneh C.M., Mangalagiu I.I., Danac R., Phys. Sci. Rev. 8(9), 2583-2645 (2023);

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KN21

The cycloaddition of benzimidazolium ylides to alkynes: the mechanism elucidation

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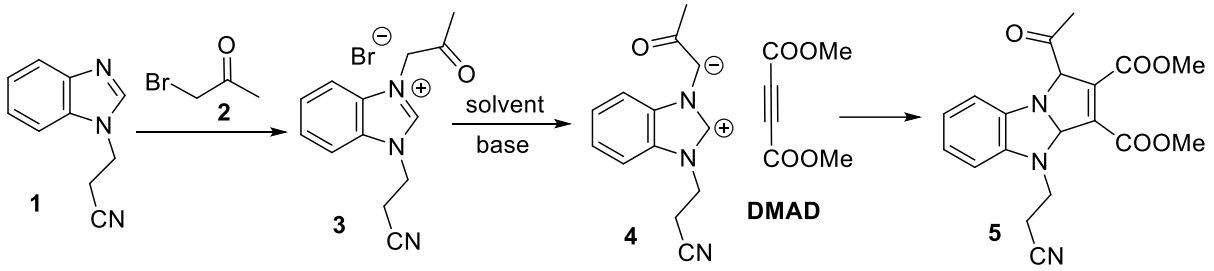
The synthesis of indolizines and azaindolizines has attracted mounting interest in recent years, driven by a broad spectrum of potential applications, ranging from electroluminescent materials to macrocyclic fluorescent sensors [1, 2]. Of particular interest are pyrroloimidazole (PD) derivatives, which exhibit a highly efficient blue fluorescence emission [3], rendering them attractive materials in optoelectronics for blue organic light-emitting diodes.



The construction of fluorescent PD derivatives is typically accomplished through the utilisation of the Kröhnke salt method [4]. Consequently, benzo[d]imidazolium salt **3** was synthesised by the reaction of 3-(1H-benzo[d]imidazol-1-yl)propanenitrile **1** with bromoacetone **2**. In the process of synthesising highly fluorescent pyrroloimidazole derivatives **5**, a [3+2] dipolar cycloaddition of benzo[d]imidazolium ylides **4** was employed. These ylides **4** were generated *in situ* from the corresponding cycloimmonium salts, in the presence of DMAD. In this study, the impact of the reaction conditions, specifically the solvent and base, on the aromatization of the cycloaddition products is investigated.

Keywords: ylide, cycloaddition, benzimidazol.

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References

1. Valeur, B., Molecular Fluorescence, Ed. Wiley-VCH, Weinheim, (2002).
2. Thompson, M.A., Forrest, S.R., Nature 403, 750, (2000).
3. Mitsumori, T., Bendikov, M., Sedo, J., Wudl, F., Chem. Mater. 15, 3759, (2003).
4. Krohnke, E., Ber. Dtsch. Chem. Ges. 68, 1177, (1935).

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KN22

Advancing the electromechanical performance of silicone dielectric elastomers

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Emerging technologies such as robotics, wearable devices, prosthetics, and renewable energy systems increasingly require actuators, sensors, and energy harvesters that are lightweight, flexible, and capable of seamless integration into soft or adaptive structures. Dielectric Elastomer Transducers (DETs) offer a unique combination of mechanical compliance, large strain capability, and electro-mechanical coupling that directly addresses these needs. DETs are able to respond to mechanical (sensing, energy generation) or electrical (actuation) stimuli.

A high dielectric permittivity, low dielectric loss, and well-controlled mechanical properties are required for DET applications. One of the main reasons for using silicones in DETs is their high flexibility and low Young's modulus, which allow for considerable mechanical deformations. High dielectric strength, unusual rheological properties associated with highly elastic behavior, very low glass transition temperature (Tg), ability to maintain functional properties, as well as store energy, over a wide range of frequencies and temperatures are all displayed by silicone elastomers. Performance of the DETs is limited by silicone elastomers' low relative permittivity. Enhancing this feature without sacrificing silicones' other advantages is the main goal of current attempts. One approach involves chemically modifying silicones with various dipoles or using additives that improve dielectric properties. The characteristics of the siloxane polymer (chain microstructure and length), the pattern and degree of crosslinking, as well as additional factors, such as the type and amount of filler or the presence of rigid and/or polar groups, significantly influence the mechanical properties. Our latest attempts in this field, which involve either physically inserting polar compounds (e.g., POSS, metal complexes, organic polymer nanoparticles, etc.) or chemically modifying polysiloxanes with various polar groups (cyanopropyl, carboxypropyl, aminopropyl, chloropropyl, etc.) into silicone matrices, subsequently crosslinked by appropriate mechanisms, are discussed and critically examined.

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KN23

Crystal engineering of azulene-based organic and metal-organic cages

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Organic cages have attracted considerable attention as molecular materials with potential applications in gas storage, molecular recognition, and catalysis [1]. Among the available synthetic strategies, the Schiff-base condensation of amines and aldehydes is particularly attractive because it provides access to diverse cage architectures and allows straightforward purification. Despite significant progress in this field, controlling the stoichiometry and geometrical features of the assemblies remains a challenge [2]. Even small changes in reaction conditions, such as solvent, concentration, reagent structure, or order of addition, can dramatically influence the final topology of the assemblies [3].

We examined the Schiff-base condensation of azulene-1,3-dialdehyde with two triamine linkers, namely tris(2-aminoethyl)amine (TREN) and 1,3,5-tris(aminomethyl)-2,4,6-triethylbenzene (TAMTMB) [4.5]. The reaction of the dialdehyde with the flexible tertiary amine, TREN, yielded the cationic $[1+1]^{2+}$ tetraimine cage and cyclic hexaimine cage, depending of the reactants stoichiometry and the presence or absence of the trifluoroacetic acid. In the case of the hexaimine cage, a conformational arrangement was observed in solution owing to flexible, aliphatic arms of TREN. Through complexation of silver ions, conformational change occurred, with the formation of a metallacage that assembles into a supramolecular network with a honeycomb topology *via* π-π stacking interaction between azulene moieties [5]. When 1,3,5-tris(aminomethyl)-2,4,6-triethylbenzene (TAMTMB) was used, the condensation reaction leads to the formation of a hexaimine cage, in which the the phenyl units form the 'floor' and 'roof' of the central cavity. The cage exhibits poor solubility in lipophilic solvents and undergoes rapid hydrolysis in slightly acidic deuterated solvents. Reduction of the cage with $NaBH_4$ gave the corresponding stable macrobicyclic hexaamine in almost quantitative yield [6]. Owing to the azulene motif, these organic cages are redox active and show fluorescent properties, highlighting their multifunctionality.

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References

1. Yang, X.; Ullah, Z.; Stoddart, J. F.; Yavuz, C. T., Chem. Rev. 2023, 123, 4602.
2. Briggs, M. E.; Cooper, A. I., Chem. Mater. 2017, 29, 149.
3. Liu, X.; Warmuth, R., J. Am. Chem. Soc. 2006, 128, 14120.
4. Ion A. E., Maxim C., Hanganu A., Dogaru A., Madalan A. M., Novikov A. S., Shova S., Andruh A., Nica S., Cryst. Growth Des. 2025, 25, 1743.
5. Ion A. E., Dogaru A., Maxim C., Hanganu A., Enache C., Andruh A., Nica S., Synthesis, 2025, 57, 2189.

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KN24

MXene-based catalysts for selective oxidation of methane at low temperatures

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The development of efficient catalysts for the low-temperature oxidative conversion of methane into valuable chemicals remains a major scientific challenge. Two-dimensional transition metal carbides—MXenes—have emerged as promising candidates due to their unique properties, including high electronic conductivity, hydrophilicity, and stability against chemical degradation and oxidation at elevated temperatures. [1, 2]. These features are attributed to their rich surface chemistry, developed during wet-etching synthesis, which introduces reactive −O and −OH functional groups.

In this study, we report a novel catalytic system using $Ti_3C_2T_x$-MXene as a support for VO_x species to selectively oxidize methane into formaldehyde at low temperatures and ambient pressure, with molecular oxygen as the oxidant. The catalyst was extensively characterized using XRD, Raman spectroscopy, SEM, TEM, transient operando XPS, and DRIFTS, revealing critical insights into its structure–activity relationships.

The strong synergy between the MXene support and the oxide phase, along with the 2D architecture of $Ti_3C_2T_x$, enables a formaldehyde selectivity of 70% at 250 °C under ambient pressure. This high level of selectivity is closely linked to dynamic changes in the catalyst's surface composition during the reaction, offering important clues about its mechanism of action. Notably, when the catalyst is exposed to a CH_4/O_2 (1:1) gas mixture at 250 °C, pronounced alterations in surface chemistry were detected, emphasizing the critical role of surface oxygen species.

The insights gained from this study contribute to the fundamental understanding of catalyst behavior and serve as a foundation for the rational design and optimization of next-generation catalysts for low-temperature oxidative transformations.

References

1. I. M. Chirica, A. G. Mirea, Ş. Neaţu, M. Florea, M. W. Barsoum, F. Neaţu, Journal of Materials Chemistry A, 35, 19589 (2021)
2. M. M. Trandafir, F. Neaţu, I. M. Chirica, Ş. Neaţu, A. C. Kuncser, E. I. Cucolea, V. Natu, M. W. Barsoum, M. Florea, ACS Catalysis 10, 5899 (2020)

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KN26

Meat analogues: A sustainable solution for future food systems

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Growing consumer concern about food choices and their potential impact on health and the environment has led to noticeable changes in eating habits, including a reduction in meat consumption. This shift reflects an increasing awareness of the importance of adopting plant-based diets—especially meat analogs—driven by ethical concerns and the rising levels of greenhouse gas emissions associated with animal agriculture, which are harmful to the environment. Informing consumers about the health benefits of meat analogs made from sustainable sources—rich in plant-based proteins, essential amino acids, and low in fat, especially saturated fat, and free of cholesterol—alongside accurate views on environmental protection and the adoption of emerging food production techniques, is expected to lead to a significant increase in the market for this segment in the near future.

The aim of this study was to investigate meat analogs produced by high-moisture extrusion from blends of pea protein isolate mixed in a 1:1 ratio with soryz flour, chickpea flour, and hazelnut flour, processed under two distinct heating temperature profiles, maxim of 100 ºC and 120 ºC. The study evaluated physicochemical properties, texture, color parameters, protein digestibility, and antioxidant activity of the products, including simulated in vitro gastrointestinal digestion following standardized methods. The results showed that both the type of plant-based raw material and the extrusion heating temperature profile had a significant impact on the quality attributes of the meat analogs. Higher processing temperatures led to a slight decrease in the nutritional compound content of the final products. All samples exhibited good water and oil retention capacities. Furthermore, extrusion at elevated temperatures caused an increase in hardness, likely due to protein denaturation and aggregation, resulting in a firmer texture. Protein digestibility of the processed meat analogs ranged between 69.37% and 86.84%. Aantioxidant activity decreased slightly in the extruded samples. Color parameters were significantly affected by both the color of the raw materials and the extrusion conditions. Higher extrusion temperatures produced darker products as a result of Maillard reactions and caramelization. Principal component analysis was employed to investigate the relationships among physicochemical characteristics, protein digestibility, antioxidant activity, texture profile, and CIELab color parameters of these high-moisture meat analogs.

This analysis emphasizes that addressing the challenges related to raw material selection and emerging processing technologies, while aligning with consumer preferences and socioeconomic opportunities, is crucial for the successful market adoption of meat analogs.

Acknowledgements
Moldovan-Turkish Bilateral Projects 23.80013.5107.3TR, “Sustainable Nutrient-Rich New Generation Food Products Development: evaluating the relationship between ingredients, processing methods used, and techno- and bio-functional properties” and and Institutional Project 020405 “Optimizing food processing technologies in the context of the circular bioeconomy and climate change”, Bio-OpTehPAS, being implemented at the Technical University of Moldova.

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KN27

Fully inkjet-printed transition metal dichalcogenide FET biosensors for express *E. coli* detection

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Foodborne pathogens continue to represent a major global health challenge, with Escherichia coli (*E. coli*) being one of the most common causes of severe gastrointestinal infections and outbreaks. Traditional detection methods such as PCR and ELISA, while highly specific, remain time-consuming, costly, and dependent on specialized laboratory infrastructure. This creates a critical need for portable, cost-effective, and rapid biosensing devices that can be deployed at the point of need. Field-effect transistors (FETs) are ideal candidates for such applications because their operation is based on changes in electrical conductance when target biomolecules bind to its surface [1] (Fig. 1). This real-time detection mechanism provides high sensitivity, scalability, and integration potential with portable platforms - features that are particularly attractive for pathogen monitoring.

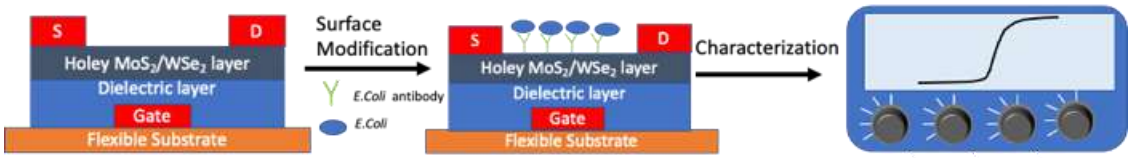

Figure 1. A schematic of the fabrication of TMD-FET by inkjet printing and their functionalization.

In this collaborative project between Moldova State University and Istanbul Technical University, we explore the fabrication of fully inkjet-printed FET biosensors using two-dimensional transition metal dichalcogenides (TMDs) [2]. In this work a successful synthesis of monolayer MoS_2 and WSe_2 crystals were achieved - development of high importance, as the monolayer form of TMDs provides superior electronic compared to their multilayered counterparts, including a direct bandgap and enhanced charge carrier mobility, that are both crucial for achieving sensitive and reliable biosensing performance.

Our approach incorporates defect (hole) engineering in the basal planes of these TMDs, improving both ink stability for the printing process and providing additional active sites for antibody immobilization. Preliminary results suggest promising behavior in terms of reproducibility and potential sensitivity. Importantly, the use of fully inkjet-printed architectures highlights a pathway towards low-cost, scalable, and flexible biosensing devices that could be potentially adapted to detect not only *E. coli* but also a large variety of pathogens. This study therefore represents an integration of advanced nanomaterials with digital fabrication techniques, bringing biosensor technology closer to real-world applications in food safety and healthcare monitoring.

References

1. Manimekala T., et al. Nanomaterial-Based Biosensors using Field-Effect Transistors: A Review. J. Electron. Mater. 51, 1950–1973 (2022)
2. Sun H., et. al. A Review of Transition Metal Dichalcogenides-Based Biosensors. Front. Bioeng. Biotechnol. 10:941135 (2022)

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KN28

Anti-glioblastoma activity and singlet oxygen generation of novel imidazole-based tetrachloroferrates

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Tetrachloroferrate-based compounds are known for their anticancer properties [1,2]. Singlet oxygen ($^1O_2$) from triplet oxygen ($^3O_2$) is a very reactive molecular oxygen species and widely used for the synthesis of chemicals and of biologically or pharmacologically active compounds [3]. Here, we report newly synthesised imidazole-derived tetrachloroferrate(III) salts (compounds **8**–**11**, Figure 1) with dual properties as photosensitizers and selective anticancer agents.

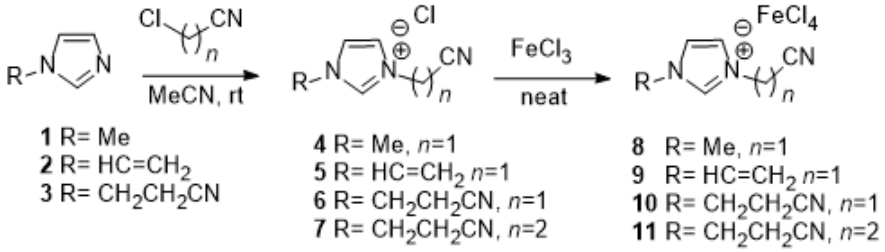

Figure 1. Synthesis of imidazole-based tetrachloroferrates **8**–**11**.

$^1O_2$ generation was confirmed by ESR spectroscopy using TMP-OH as a spin trap. Upon UV irradiation, strong signals were observed, particularly for compounds **10** and **11**, indicating efficient $^1O_2$ production in aqueous suspensions. These results were corroborated by photodegradation experiments with bisphenol A, where >80% degradation was achieved.

The compounds were tested against a panel of tumour cell lines. Strikingly, they displayed selective cytotoxicity only against LN229 glioblastoma cells, with IC_{50} values of 1.0–4.0 μM, comparable to etoposide, while showing negligible activity (IC_{50} > 100 μM) against other solid and haematological cancers. Importantly, the compounds were far less toxic to peripheral blood mononuclear cells (IC_{50} = 10.3–59.8 μM), suggesting a favourable therapeutic window. Additional assays showed no significant effects against U87 MG or U138 MG glioblastoma lines, likely reflecting genetic differences, including mutant versus wild-type p53 status.

In conclusion, imidazole-based tetrachloroferrate(III) salts act as efficient $^1O_2$ generators and show selective activity against LN229 glioblastoma cells. Their unique dual functionality supports further investigation as candidates for targeted anticancer or photodynamic applications.

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References

1. Y. Qi, E. Miyako *Small Sci*. **2025**, *5*, 2400640; [2] V. Boldescu, N. Sucman, S. Hassan, J. Iqbal, M. Neamtu, J. Lecka, J. Sévigny, D. Prodius, F. Macaev, *ChemMedChem*, **2018**, 13, 21, 2297-2304. [3] I. Pibiri, S. Buscemi, A. Piccionello, A. Pace, **2018**, 2(7) 535-547.

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ORAL PRESENTATIONS

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OL1

Reusable zwitterionic ion-exchange resins for the removal of heavy metals from contaminated water

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Environmental contamination by heavy metal ions (HMIs) has intensified due to expanding industrial activities such as mining, metallurgy, and chemical manufacturing [1]. With properties including high selectivity, adaptability, and the ability to be reused, ion exchange resins (IExRs) serve as promising materials for the removal of HMIs from contaminated water sources. The removal mechanism is based on the exchange of counter-ions in the resin with target metal ions in the solution [2]. Through chemical modification, these materials acquire desirable physical and chemical properties, such as enhanced hydrophilicity, incorporation of specific chelating functional groups, and tunable porosity [3]. Among these modifications, functional groups such as amino/imino (–NH_2/–NH–), carboxyl (–COOH), and amide (–NH–CO) have shown strong potential for donor-acceptor interactions, enabling selective binding with divalent and trivalent metal cations [4].

In this study, IExRs were synthesized via the copolymerization of ethyl acrylate, acrylonitrile, and 8% divinylbenzene as a crosslinker, followed by functionalization with ethylenediamine and triethylenetetramine or hydrazine hydrate to yield weak cationic resins bearing amino groups. Also, the formation of zwitterionic resins via reaction of the weak cationic resins with sodium chloroacetate was followed. The structures and morphologies of the synthesized resins were characterized using infrared spectroscopy and scanning electron microscopy.

The sorption performance of IExRs was evaluated through batch experiments using mono- and multicomponent aqueous solutions of Cu(II), Fe(II), and Mn(II) ions, as well as a water sample collected from the Tarnita area. Following IExR sorption, the concentration of HMIs was reduced to below the permissible limits for surface water. The waters toxicity was assessed using wheat germination, revealing harmful effects of the untreated Tarnita water, while the treated supernatant showed no toxic impact. The study represents a significant step toward addressing the environmental issues in the Tarnita closed mine area by enabling the removal of major contaminants from the polluted local river water.

Acknowledgements: This work was financially supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS-UEFISCDI, project number PN-IV-P1-PCE-2023-0738, within PNCDI IV.

References

2. Sharafi S., Salehi F. Scientific Reports, 15(1), 7518, 2025.
3. Zaharia, M.M., Vasiliu, A.L., Trofin, M.A., Pamfil, D., Bucatariu, F., Racovita, S., Mihai, M. Reactive and Functional Polymers, 166, 104997, 2021.
4. Zaharia, M.M., Bucatariu, F., Vasiliu, A.L., Mihai, M. Chemosphere, 304, 135383, 2022.
5. Zaharia, M.M., Bucatariu, F., Vasiliu, A.L., Mihai, M. ACS Applied Polymer Materials, 5(10), 8183-8193, 2023.

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OL2

Hybrid nanostructures based on AMP-*g*-PAA as mediator for *in situ* gold nanoparticles

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Gold nanoparticles (AuNPs) are submicrometer-sized gold particles that exhibit localized surface plasmon resonance properties and possess advantageous properties, such as being inert, biocompatible, and non-toxic, making them ideal for a broad spectrum of applications, including biosensing, drug delivery, photomedicine and vaccine development [1,2]. The use of hybrid macromolecular materials based on polysaccharides and stimuli-responsive polymers as stabilizing and coating agents for AuNPs, represents a promising approach for the development of smart/responsive hybrid nanomaterials, that integrate their functionalities and properties. Inspired by this requirement, the overall objective of this study was the synthesis and characterization of a new hybrid copolymer based on amylopectin (AMP) and poly(acrylic acid) (PAA), followed by the synthesis of AuNPs mediated by AMP-*g*-PAA and their characterization.

The synthesis of the AMP-*g*-PAA copolymer was performed first by synthesis of PAA by reversible addition-fragmentation chain transfer (RAFT), and then the anchoring of PAA chains to the backbone of AMP following the "grafting to" technique. In the next step, the hybrid composites of AMP-g-PAA and AuNPs were prepared following an *in situ* thermally assisted process, in aqueous solution, using $HAuCl_4$ and AMP-*g*-PAA copolymer in different molar ratios, without using any other reducing agents.

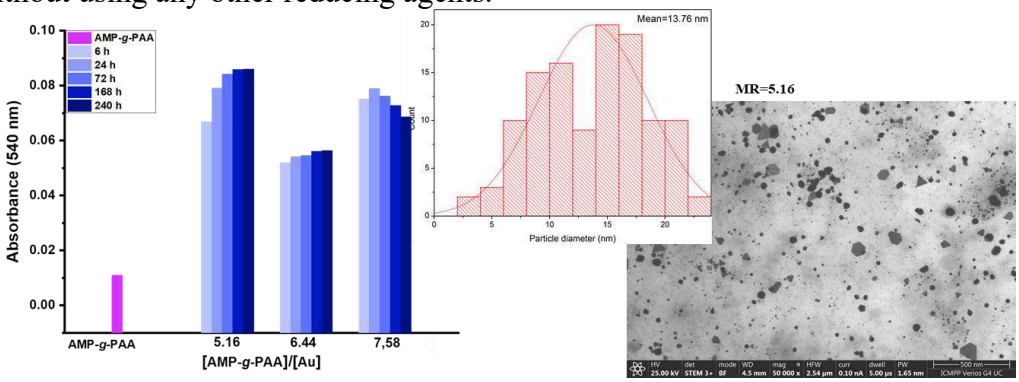

Figure 1. The change in the absorbance at 540 nmin the UV-Vis spectra of as a function of the molar ratio (MR) AMP-g-PAA/Au for AuNPs formed at 60ºC and the STEM micrographs at 500 nm scale bar (MR = 5.16, 60 ºC)

To investigate the kinetics of hybrid composites synthesis in relation to reaction temperature and MR, UV-Vis measurements, dynamic light scattering (DLS) and scanning transmission electron microscopy (STEM) were performed. Summarizing, the synthesis of AuNPs using AMP-*g*-PAA has the best eficiency at 60 ºC and molar ratio of 5.16 (Figure 1).

Acknowledgements: This work was supported by the Romanian National Authority for Research, by project HYBSAC, project number PNRR-III-C9-2022-I8-201, within the National Recovery and Resilience Plan.

References

1. Tepale N, Fernández-Escamilla VVA, González-Coronel VJ., Luna-Flores A, Aguilar J., Carreon-Alvarez C., Carreon-Alvarez, A. Crystals, 9, 612, 2019.
2. Sarkar AK, Mandre NR, Pandac AB, Pal S. Carbohydr. Polym. 95, 753–759, 2013.

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OL3

Mechanistic insights into the turn-Off/On fluorescence behavior of a PEDOT–cyclodextrin supramolecular architecture toward metal ions

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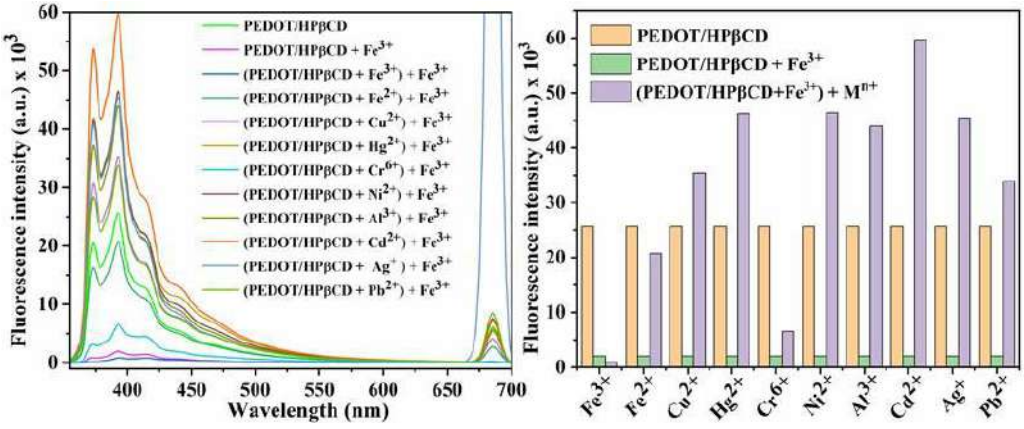
Luminescent materials have become key tools in chemical, biological, and environmental sensing due to improved optical instrumentation and advanced fluorophores with tunable responses. Among these, fluorescence-based chemosensors have emerged as powerful tools for detecting metal ions, offering high sensitivity and selectivity that are essential for monitoring toxic or biologically relevant species in environmental and medical contexts [1]. Such sensors typically exhibit one of three fluorescence response modes: intensity quenching (turn-off), intensity enhancement (turn-on), or an emission wavelength shift to a different wavelength [2].

In this work, a novel polyrotaxane system was synthesized through a supramolecular self-assembly process that integrates the conductive π-conjugated backbone of PEDOT threaded by HPβCD macrocycle molecules and was characterized by UV-Vis and fluorescence spectroscopy. The material exhibited dual fluorescence behavior in the presence of various metal ions. A pronounced fluorescence quenching effect (-95.66%) was observed upon addition of Fe^{3+} ions, indicating strong interaction with the conjugated backbone, while Cd^{2+} ions induced a remarkable fluorescence enhancement (+103.43%), attributed to coordination-induced restriction of non-radiative decay pathways. These contrasting optical responses demonstrate the system's dual sensing capability. Further investigations regarding quenching mechanism, detection limits, selectivity, fluorescence quantum yield, complex stoichiometry, and association constants confirm its potential as a selective and sensitive fluorescent chemosensor for metal ion detection.



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References

1. Callan, J.F.; Silva, A.P.D.; Magri, D.C., Luminescent sensors and switches in the early 21st century. Tetrahedron, 61 (2005), 8551–8558.
2. Bui, T.H.; Thangadurai, D.T.; Sharipov, M.; Nghia, N.N.; Cuong, N.V.; Lee, Y.-I., Recent advances in turn off–on fluorescence sensing strategies for sensitive biochemical analysis – A mechanistic approach. Microchemical Journal, 179 (2022), 107511.

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OL4

Phospha(chalcogenoxo)phosphoranes, rich-electron building blocks for new organometallic and coordination compounds

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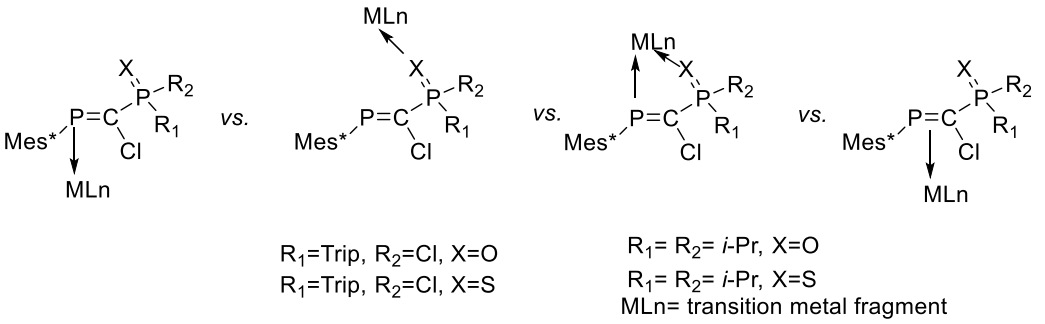
Transition metal compounds with organophosphorus ligands containing a RP=CR_2 (phosphaalkene) or a RP=C(R)–PR_2 (phosphavinylphosphoranes) unit are interesting due to their possible catalytic activity.[1] Several metal complexes of Ru, Rh, Ir, Ni, Pd and Pt, containing such ligands have shown promising results in various processes. The multiple coordination possibilities of phosphavinylphosphoranes that have a P(III)=C–P(V)(=X) (X= O, S), such as the electron lone pair at the level of the phosphorus or the chalcogen atom, as well as the π(P=C) bond, make these systems seem very attractive for the preparation of novel organometallic or coordination compounds with metal centres that could lead to interesting properties.



We hereby present a study regarding the coordination ability of compounds with the general formula Mes*P═C(Cl)–P(=S)R_1,R_2 (Mes* = 2,4,6-tri-*t*-butylphenyl; R_1 = Cl, R_2 = 2,4,6-tri-*i*-propylphenyl; R_1 = R_2 = *i*-propyl) with transition metal fragments containing Au, P, and W, evaluated by means of experimental and theoretical investigations.[2] The nature of the organic groups or atoms attached to the sp^3 phosphorus atom involved in the bonding to the metal centre influences the preferred coordination mode. The targeted compounds were characterized in solution by multinuclear NMR spectroscopy and HRMS, while for several cases, the solid-state structures were measured through X-ray diffraction.

References

1. Ziółkowska, A., Szynkiewicz, N., Ponikiewski, Ł. Organometallics, 2023, 42, 505-537, DOI: 10.1021/acs.organomet.2c00379
2. Aghion, I.-A., Septelean, R, Tomut, A.-C., Moraru, I.-T., Soran, A., Nemes, G., Organometallics, 2024, 43, 2062-2076, DOI: 10.1021/acs.organomet.4c00270.

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OL5

Porphyrin is mightier than corrin: reactivity tales of two tetrapyrroles

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Metal ligation is central in biochemistry because it fine-tunes both the structure and the reactivity of enzymes and their cofactors.

Porphyrins are ancient cofactors that almost certainly predate the Great Oxygenation Event. They are among the most important ligands in biochemistry because they provide a highly versatile, finely tunable, and robust platform for several essential biological functions such as oxygen transport, cellular respiration, and redox catalysis. Heme is particularly suited to generate high-valent iron intermediates, such as Compound I and Compound II, which are among nature's most potent oxidants. Despite the stabilization brought by complexation, heme iron can still engage in Fenton-like reactions to generate free radicals.[1]

Corrins are another type of more specialized tetrapyrrole ligand. As the cofactor of cobalamin, corrin is required for a small number of enzymes that catalyze unique reactions, such as methyl transfers and radical rearrangements. As opposed to porphyrins, corrins could support the generation of low-valent metal intermediates.[2]

In this work, we explore the reactivity of heme proteins (horse heart myoglobin, truncated hemoglobin 3 from *A. thaliana*, and cytochrome P450) in their various oxidation state (ferrous, ferric, high-valent iron) towards small molecules such as nitrite, hydrogen peroxide[3], and cyanide/cyanamide[4]. We also evaluate the ability of heme centers to engage in Fenton-like processes.[5,6] To spice things up, we draw a comparison to cobalamin[7,8] and rationalize the differences in reactivity. Is porphyrin indeed mightier than corrin?

Acknowledgments
This work was supported by the projects ”Programul 5.8 – Cooperare europeană și internațională: Proiecte complexe bilaterale cu Republica Moldova”, contract no. 52PCBROMD/2025, code PN-IV-PCB-RO-MD-2024-0515, and “Targeted Tumor Therapy with multifunctional platinum(iv)-drug conjugates (T3-Pt)” funded by European Union – NextGenerationEU and Romanian Government, under National Recovery and Resilience Plan for Romania, contract no 760240/28.12.2023, code PNRR-C9-I8-CF 76/31.07.2023, through the Romanian Ministry of Research, Innovation and Digitalization.

References

1. Poulos, T.L. 2014. Chemical reviews, 114 (7), 3919-3962.
2. Padmanabhan, S., et al. 2017. Annual Review of Biochemistry, 86 (1), 485-514.
3. Zagrean-Tuza, C., et al. 2025. Journal of Biological Inorganic Chemistry, 30 (1), 61-70.
4. Zagrean-Tuza, C., et al. 2025. submitted.
5. Zagrean-Tuza, C., et al. 2020. Free Radical Biology and Medicine, 146, 189-197.
6. Zăgrean-Tuza, C., et al. 2024. Journal of Inorganic Biochemistry, 258, 112613.
7. Lehene, M., et al. 2021. Inorganic Chemistry, 60 (17), 12681-12684.
8. Lehene, M., et al. 2025. Journal of Biological Inorganic Chemistry, 30 (1), 25-34.

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OL6

Thermodynamic insights into synergistic enhancement of drug solubility

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This study introduces, for the first time in the scientific literature, the concept of *synergistic coefficient* (*SC*), developed through original mass balance (*MB*) equations adapted for heterogeneous drug *HD* – cyclodextrin *CD* – auxiliary agent *HA* (*HD – CD – HA*) systems. The key innovation lies in an additional concentration term accounting for the solid-phase drug fraction per unit volume of the heterogeneous mixture. This allows, in conjunction with existing thermodynamic data, the quantitative estimation of both the solid-phase drug content and the synergistic effect as functions of chemical composition and pH.

The methodology addresses a major challenge in pharmaceutical development: the poor aqueous solubility of many drugs, which limits their bioavailability. Cyclodextrins, known for forming noncovalent inclusion complexes with hydrophobic drugs, are widely used to enhance solubility. Incorporating a third component, such as hydroxy acids, amino acids, or metal ions, into *CD* – drug systems, yields ternary complexes that often exhibit superior solubility and stability due to cooperative interactions. The thermodynamic basis of these effects is attributed to increased complex stability constants, as observed in various systems beyond pharmaceutics, including solvent extraction and catalysis.

The introduced *synergistic coefficient* (*SC*) quantitatively expresses the degree to which an auxiliary agent enhances ($SC > 0$) or inhibits ($SC < 0$) drug solubilization in ternary systems, relative to binary complexes. *SC* values are derived from equilibrium modeling across a pH spectrum, supported by the Law of Mass Action. The full distribution profiles of drug species in both aqueous and solid phases were established using this framework. Application to ten commercial drugs, including cimetidine and flurbiprofen, demonstrated the broad utility of this approach. By integrating selected thermodynamic datasets, the quantities of drug retained in the solid phase and the magnitude of the synergistic effect can be quantitatively determined as functions of the system's composition and pH.

These findings not only advance our understanding of cooperative effects in multicomponent pharmaceutical systems but also provide a generalized thermodynamic framework applicable to a wide range of heterogeneous equilibrium systems involving poorly soluble compounds.

Acknowledgments: This work has been carried out within the Research and Innovation Program "Stimulating excellence in research", „*The thermodynamic elucidation and prediction of chemical synergism in complex chemical processes*", 2024-2025, code 20.80012.5007.19SE. A part of the work was carried out within the Institutional Research Program of the State University of Moldova for the period 2024-2027, subprogram "*Advanced Research in Computational and Environmental Chemistry, Identification of Technological Treatment Processes, Formation of Water Quality and Quantity*", code 010603.

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OL7

The power of comprehensive genetic testing in one family case

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Comprehensive genetic testing is essential for ensuring accurate prenatal diagnosis. Here, we present a case where an integrated genetic approach was essential in guiding clinical decisions.

An *in vitro* fertilization (IVF) pregnancy was established, following embryo selection by preimplantation genetic testing for aneuploidy (PGT-A). The first-trimester ultrasound revealed a 4.5 mm nuchal translucency, prompting chorionic villus sampling. Single nucleotide polymorphism (SNP) microarray on an Affymetrix 750K platform identified a 12 Mb region of absence of heterozygosity (AOH) on chromosome 6; consequently, further investigation through whole exome sequencing (WES) was recommended. Whilst no pathogenic variant was found in the AOH region, a likely pathogenic heterozygous variant in *PKD1* gene, c.1598C>G, was detected; this gene, when abnormal, leads to polycystic kidney disease type 1, with autosomal dominant inheritance. Following this genetic finding, an ultrasound examination was conducted on the fetus, resulting in the detection of characteristic features of polycystic kidney disease, thus confirming the diagnosis of autosomal dominant polycystic kidney disease (ADPKD). Subsequently, parental testing by Sanger sequencing confirmed paternal transmission, leading to an unexpected diagnosis of a mild form of autosomal dominant polycystic kidney disease (ADPKD) in the father.

This case emphasizes the value of a multilevel genetic workflow - spanning PGT-A, SNP microarray, WES, and Sanger sequencing - in securing a definitive diagnosis. It underscores the importance of providing comprehensive genetic analysis under appropriate genetic counselling, ensuring accurate risk assessment and optimized patient care.

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OL8

Unveiling wine provenance: A metabolomic and isotopic approach for discriminating neighboring vineyards

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Geographic origin, soil composition, grape variety, and viticultural practices play a fundamental role in shaping the physicochemical profile of wine, forging a strong connection between a wine and its terroir. Consumer demand for high-quality wines is rising, with purchasing decisions primarily influenced by grape variety and geographic provenance. However, the wine sector is increasingly affected by fraudulent practices such as mislabeling of botanical and geographical origin, driven by significant and often concealed economic interests—actions that mislead consumers and disadvantage genuine producers. In this context, the development of reliable analytical methods for wine authentication is of growing interest to both regulatory bodies and producers. This study evaluates the potential of proton nuclear magnetic resonance (^{1}H NMR) spectroscopy and isotope ratio mass spectrometry (IRMS) combined with multivariate statistical analysis to discriminate wine samples by grape variety, geographical origin, and vintage. The study focused on red and white wines (Merlot, Fetească Neagră, Sauvignon Blanc, Cabernet Sauvignon, Chardonnay, and Fetească Regală) commonly produced in Romania and neighboring countries, harvested over multiple vintages from neighboring vineyards within the Drăgășani region. These vineyards share similar pedoclimatic conditions but differ in slope exposure, allowing for a nuanced assessment of origin-related chemical variability. Wines were correctly classified by geographic origin with 91.89% accuracy based on key metabolites (e.g., shikimic acid, glycerol, isopentanol, sorbic acid, fumaric acid) and 81.08% accuracy based on stable isotopes, particularly δ^{13}C. For varietal classification, metabolomic profiling yielded 83.61% accuracy, with discriminant compounds such as β-glucose, alanine, fructose, sucrose, arabinose, caftaric acid, acetic acid, lactic acid, tyrosine, and choline, while stable isotope data achieved 59.46%. Vintage differentiation showed moderate separation, with fumaric acid, alanine, and δ^{18}O contributing to classification. Importantly, the discriminative power of stable isotopes must not be underestimated. Despite the proximity and overall climatic similarity of the studied vineyards, subtle isotopic differences—arising from variations in slope exposure and microclimatic conditions—provided meaningful support in origin authentication. Thus, the combined use of metabolomics and isotope ratio analysis enhances the robustness of wine authentication strategies in viticultural regions with fine-scale environmental heterogeneity.

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OL9

NMR insights in tomatoes degradation

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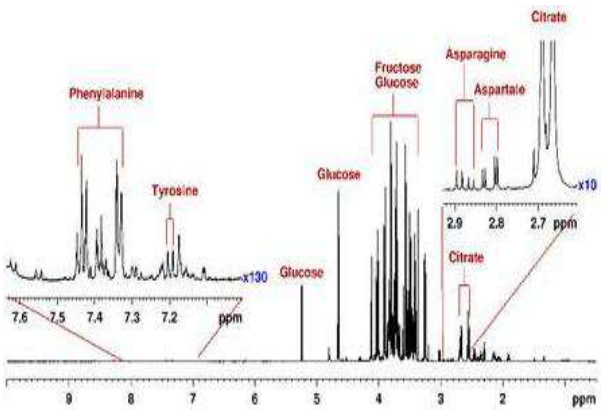
Tomato (Solanum lycopersicum) is one of the most produced vegetables in the world, with 189 million tons in 2021 [1]. The industrial processing of tomatoes generates a large amount of waste on which metabolomic studies could be done in order to characterizing it and monitor its evolution in time.

Metabolomics of tomatoes became an important topic in recent years due to the existence of a large number of varieties, both natural and genetically modified.

NMR spectroscopy has proven to be one of the most versatile techniques for characterization of primary metabolites in ex vivo matrices of vegetal fluids. Although there are some previous metabolomic characterizations of several tomatoes' varieties, up to date there is no dynamic metabolomic characterization of tomatoes' degradation in various conditions. The vegetables' degradation metabolomics is of fundamental importance for the study of metabolic mechanisms but it is also important for the applied agro-food sector in determination of shelf life of commercial products and for the characterization of biological material for possible vegetable waste recycling.

In the present study we followed the metabolism of tomatoes' degradation in various aeration conditions. Figure 1 exemplifies the ^{1}H NMR spectrum of sample of fresh tomato juice.

The reproducibility of NMR instruments used for metabolomic studies was also assessed [2].



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References

1. Food and Agriculture Organization of United Nations, Agricultural production statistics 2000-2021, FAO (2021).
2. Stavarache C, Nicolescu A, Duduianu C, Ailiesei GL, Balan-Porcăraşu M, Cristea M, Macsim AM, Popa O, Stavarache C, Hîrtopeanu A, Barbeş L, Stan R, Iovu H, Deleanu C (2022) A Real-life Reproducibility Assessment for NMR Metabolomics. Diagnostics 12: 559.

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OL10

HPV cervical screening performans in LMICs: Results, oportunities, priorities, meta-analyses

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Meta-analysis: HPV self-sampling vs provider-collected sampling in LMICs
Introduction: Global cervical cancer elimination strategies emphasis screening uptake alongside high-quality tests. In low- and middle-income countries (LMICs), barriers such as clinic access, cultural norms, and provider shortages limit screening participation. Self-sampling for HPV testing (i.e., women collect their own specimen) has emerged as a promising innovation to expand reach. Yet evidence on its effect on uptake and cost-effectiveness in LMICs remains limited. A meta-analysis was therefore conducted to assess whether self-sampling improves screening uptake compared with provider-collected samples.
Objective: To compare screening uptake and cost implications of HPV self-sampling versus provider-collected sampling in women in LMICs.
Materials and Methods: A systematic review and meta-analysis identified randomised trials in LMICs (up to April 2022) comparing HPV self-sampling versus provider-collected screening. Databases (PubMed, Embase, CINAHL, CENTRAL, Web of Science, ClinicalTrials.gov) were searched; six trials (29,018 participants) met inclusion. The main outcome was uptake (proportion screened); secondary cost data were extracted where available.
Results: In the primary analysis of six trials (29,018 participants), self-sampling yielded a modest but statistically significant increase in uptake (RR 1.11; 95 % CI: 1.10-1.11; $I^2 = 97\%$). In a sensitivity analysis excluding one heterogenous trial (5 trials; 9,590 participants), the effect was larger (RR 1.82; 95 % CI: 1.67-1.99; $I^2 = 42\%$). Two trials reported cost data; one indicated self-sampling was more cost-effective than VIA despite higher test costs.
Conclusions: HPV self-sampling in LMICs appears to significantly improve screening uptake compared with provider-collected sampling, particularly when uptake barriers are high. Limited cost data suggest potential cost-effectiveness in certain settings, but evidence remains scant. Self-sampling offers a promising opportunity to expand reach of cervical screening and address participation gaps; further large-scale trials with cost and equity analyses are needed to inform national-scale implementation.

Key words
HPV self-sampling; screening uptake; LMIC; cost-effectiveness; cervical cancer

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OL11

Genotype-phenotype relationships in the management of children with dilated cardiomyopathy

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Introduction. Dilated cardiomyopathy (DCM) is the most common cardiomyopathy phenotype, characterized by dilation and systolic dysfunction of the left ventricle. The prevalence of pediatric DCM is 0.57-1.13/100,000 children. The genotype influences the phenotype and the patient's approach.

The objectives of the study aimed to analyze current knowledge regarding the importance of genotype-phenotype relationships in the diagnosis and treatment of children with DCM.

Material and methods. We used the electronic databases PubMed, ScienceDirect, Embase, Cochrane, with the selection of scientific publications and clinical guidelines from the last 10 years.

Results and discussions. Recent guidelines (*2023 ESC Guidelines for the management of cardiomyopathy, 2023 AHA Scientific Statement*) recommend a multidisciplinary approach to patients with DCM of any age from the perspective of two objectives: (1) establishing the phenotype and (2) identifying the genotype. Human genome sequencing is now available and accessible, but data interpretation remains a challenge. The goal of treatment is to improve symptoms of heart failure and ventricular dysfunction. Study data suggest that certain genes can predict the evolution of a specific clinical phenotype. Known genotypes with a high risk of sudden cardiac death are *LMNA*, truncated variants of *FLNC* and *TMEM43*. Patients with these genotypes require cardioverter defibrillator (CDI) implantation at any age. Another challenge is the development of indication criteria and duration of medication for asymptomatic patients at risk of the disease. Understanding the particular molecular mechanisms in pediatric DCM allows for objective stratification of vital risks and selection of personalized treatment.

Conclusions. In the multidisciplinary approach to children with DCM, the interaction between cause, onset and clinical evolution will be taken into account, and determining the genotype-phenotype relationship allows for the selection of personalized treatment.

Keywords: dilated cardiomyopathy, genotype, phenotype, child

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OL12

Optimization and kinetic evaluation of catechol degradation in aqueous solutions using homogeneous processes

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Catechol is widely used in various industrial applications, including photographic developers, lubricant oils, polymerization inhibitors, and pharmaceuticals. Consequently, wastewater from these industries is often contaminated with catechol. Globally, catechol is one of the most abundant phenolic pollutants in olive mill effluents. Its removal from wastewater is of critical importance due to its aromatic structure, which contributes to its toxicity and environmental persistence. The International Agency for Research on Cancer (IARC) classifies catechol as a possible human carcinogen (Group 2B), and it is listed as a hazardous substance under EU Directive 67/548/EEC, amended by Directive 2006/121/EC.

This study aimed to evaluate and optimize the operational parameters of Fenton and Photo-Fenton oxidation processes for the efficient degradation of catechol, a phenolic pollutant frequently encountered in industrial wastewater. The experimental methodology involved systematic variation of pH, concentrations of hydrogen peroxide and ferrous ions (Fe^{2+}), type of UV radiation, and stoichiometric ratios of reagents to determine their impact on degradation efficiency and reaction kinetics.

The optimal pH range for both Fenton and Photo-Fenton processes was identified as 2.6–3.2, ensuring maximum hydroxyl radical efficiency and minimal side reactions. A hydrogen peroxide concentration of 0.1 mM enabled effective degradation (~73% within 90 min under UV-C irradiation) without inducing radical scavenging effects. Similarly, 0.1 mM Fe^{2+} ensured an optimal balance between radical generation and inhibition from Fe^{3+} accumulation. UV-C radiation proved significantly more effective than UV-A in sustaining the Photo-Fenton cycle via enhanced Fe^{2+} regeneration. The optimal molar ratio of H_2O_2 : Fe^{2+}: catechol was established as 10 : 1 : 2.

Kinetic analysis revealed pseudo-first-order behavior, with the highest rate constant (0.00347 min^{-1}) and lowest half-life (~200 min) achieved in the Photo-Fenton (UV-C) system. The reaction rate reached $9.23 \cdot 10^{-8}$ mol/L·s. Among the tested methods, Fenton/UV-C demonstrated superior performance in both catechol degradation and COD reduction, indicating advanced mineralization. A hypothetical degradation mechanism can involve OH• attack on the aromatic ring, quinone formation, ring opening, and generation of low-molecular-weight carboxylic acids, ultimately leading to complete mineralization to CO_2 and H_2O.

The experimental results confirm the efficiency of the UV-C assisted Fenton process as an advanced method for the treatment of synthetic wastewater containing phenolic compounds such as catechol. The favorable synergy between operational parameters and kinetic performance supports the implementation of homogeneous advanced oxidation technologies for industrial wastewater purification. These findings provide a solid scientific basis for the development of scalable, high-efficiency treatment strategies applicable to real wastewater conditions.

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OL13

Caries risk assessment in children with congenital heart defects: perspectives on oral and systemic health

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Introduction. Congenital heart defects (CHDs) are currently a major public health problem, associated with high morbidity and mortality rates, and their incidence continues to increase worldwide. In children with CHD, the presence of chronic odontogenic infectious foci, including carious lesions, can significantly increase the risk of infective endocarditis (IE), a severe and potentially lethal complication. The role of Streptococcus mutans is widely recognized in cariogenesis, and this bacterium has also been identified in the heart valves and blood of patients with IE. Thus, assessing the risk of caries in children with CHD is particularly important both for preventing systemic infectious complications and for improving their quality of life.

The objective of the study was to assess the cariogenic risk in children with congenital heart malformations.

Research material and methods. A case-control clinical study was conducted on a sample of 98 children aged between 7 and 18 years. The children included in the study were divided into two groups of identical structure. The research group (Gr1) consisted of 49 children with CHD. The control group (Gr0) consisted of 49 healthy children. Caries risk assessment was performed using *Cariogram software* and assessment of the number of Streptococcus mutans in saliva using the *Salivar Check Mutans Kit*. Statistical analysis was performed using EpiInfo software.

Results. The caries risk estimated with *Cariogram software* was 31.04% higher in children with CHD compared to controls. The main contributing factors identified were the impact of heart disease and associated medication (particularly diuretic-induced reduction in salivary flow), poor oral hygiene, salivary *Streptococcus mutans* level $>5\times10^5$ CFU/mL, and the absence of appropriate preventive measures.

Conclusions. Children with congenital heart defects (CHD) have a significantly increased risk of caries, caused by poor oral hygiene, high salivary bacterial load with Streptococcus mutans, and the effects of diuretic treatment on salivary flow. These findings highlight the need to integrate predictive caries risk assessment into the overall management of patients with CHD as part of a comprehensive prevention strategy. The implementation of personalized oral care protocols could contribute to reducing the incidence of infectious complications, including infective endocarditis, optimizing oral health, and improving quality of life. The results also highlight the importance of close multidisciplinary collaboration between pediatric cardiology specialists and dentists for an integrated and effective approach to this vulnerable population.

Keywords: dental caries, congenital heart defects, caries risk, Streptococcus mutans, Cariogram.

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OL14

Potential toxicolgical hazards of different types of plastic packaging

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People are exposed to synthetic chemicals in food, medicines, household and personal care products, as well as environmental pollutants. Some of these chemicals have been associated with the increasing prevalence of noncommunicable diseases. Food packaging and other articles that come into contact with food pose risks of direct exposure to chemicals, which can migrate into food, and subsequently be ingested. Despite significant efforts to reduce its use, plastic remains the most widely used packaging material today. The most commonly used materials in food packaging are polypropylene (PP), polyethylene terephthalate (PET), high- and low-density polyethylene (HDPE and LDPE), and PVC (polyvinyl chloride), which provides a barrier against oxygen and moisture. The mechanical properties of plastic materials are improved by adding additives. The purpose of the work is to assess the migration of potentially toxic components from plastic food packaging, present on the market of the Republic of Moldova. The types of plastic packaging used, their destination per food groups and potential toxicological hazards were characterized and classified, in order to test the migration of potentially toxic components into different food categories (bottled water, dairy products, oils).

Bisphenols and phthalates are two very commonly used additives. Bisphenols serve as antioxidants and UV stabilizers, while phthalates are used to increase the plasticity, flexibility, and transparency of plastic materials. These two groups of molecules are risk factors: endocrine disruptors and carcinogens, which can migrate into food that comes into contact with plastic packaging. EU and RM legislation determines the limits of some chemical substances: polymers, monomers, and food contact additives. However, the uncontrolled use of a high percentage of recyclable materials for food contact poses risks to food safety and consumers. Another group of problems consists of long-term or repeated use of packaging, failure to comply with storage conditions, which can induce accelerated migration of potentially toxic components. Microwave heating also contributes to accelerating the migration of contaminants into food. Thus, although the potential toxicological effects of many constituents of food packaging are well known, an adequate risk assessment can only be carried out by testing the migration of components under the conditions of storage, processing and consumption of food.

Keywords: food packaging, plastics, contaminant migration, bisphenols, phthalates

Acknowledgments: The research was funded within the project "Assessment of the risks associated with the migration of potentially toxic components from plastic food packaging on the market of the Republic of Moldova", ERMAP-MD, call "Stimulating excellence in scientific research", 2025-2026.

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OL15

Synthesis and cytotoxic evaluation of novel naphthoquinones as potential anticancer agents

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Cancer continues to be a leading cause of death worldwide, responsible for nearly 10 million fatalities each year. Current therapeutic approaches, such as chemotherapy, are often limited by non-selectivity, significant side effects, and the emergence of multidrug resistance (MDR) in tumours [1,2]. Naphthoquinones are a class of compounds known for a broad spectrum of biological effects and have shown the ability to selectively target malignant cells. Their anticancer potential is linked to multiple pathways, including the induction of reactive oxygen species (ROS) [3], inhibition of DNA topoisomerases [4], and activation of apoptotic processes [5], positioning them as promising candidates for multimodal cancer treatment.

The goal of this study was to investigate the cytotoxic potential and selectivity of novel naphthoquinone-based compounds against various human cancer cell lines. A series of new 1,4-naphthoquinone derivatives were synthesized using several approaches:

1. Condensation of 2-hydroxyjuglone with various aldehydes in the presence of a Hantzsch ester. The aldehydes included both aromatic and aliphatic types, of synthetic and natural origin. While aromatic aldehydes reacted as expected, some natural aldehydes led to unanticipated products.
2. Reaction of juglone with different amines in the presence of copper(I) bromide, with and without formaldehyde.
3. A multicomponent Michael-type reaction involving lawsone, aldehydes, and amines simultaneously.

Structural confirmation of the synthesised compounds was achieved *via* ^{1}H and ^{13}C NMR, IR spectroscopy, GC-MS, and elemental analysis. Selected compounds were evaluated for cytotoxic activity across eight cancer cell lines, including solid and hematologic malignancies. Cytotoxicity was tested *in vitro* against several cancer cell lines: Capan-1 (pancreatic), HCT-116 (colorectal), LN229 (glioblastoma), and several leukemic cell lines, as well as PBMC (peripheral blood mononuclear cells), using previously established protocols [6]. Some derivatives demonstrated potent activity, with IC_{50} values in the low micromolar range (1–2 μM), indicating their promise as anticancer leads.

Acknowledgements
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References

1. Mir S. A., et al., Molecules, 2022, 27, 4473.
2. Holohan C., et al., Nature Reviews Cancer, 2013, 13, 714-726.
3. Pereyra et al. Cancer Cell International, 2019, 19, 207
4. Bastow et al. Cancer Chemother Pharmacol. 2001, 47(3), 187–198
5. Liu et al. Biochem Biophys Res Commun. 2015; 466(1):103–110
6. N. Sucman et al. Steroids, 210, 2024, 109475.

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OL16

Microbiostatic activity of berry powders and extracts on microorganisms responsible for food spoilage

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Antimicrobial resistance is one of the greatest threats facing modern medicine. The pressure that antibiotics exert on pathogens is responsible for the selection of resistant strains. At the same time, it is well known that many natural compounds from plants, herbs and spices possess antimicrobial action and serve as a source of antimicrobial agents against pathogenic germs. Plant extracts represent an alternative, natural solution with antibacterial action on synthetic chemical compounds. The aim of the research was to evaluate the microbiostatic action of powders and extracts from berries and spices on microorganisms responsible for food spoilage.

The results showed that phenolic compounds from berries and red grape pomace have varied antimicrobial effects against bacteria responsible for food spoilage. Different degrees of antimicrobial sensitivity of Gram-negative (*E. coli, Salmonella* etc.) and Gram-positive (*S. aureus, B. subtilis, L. monocytogenes*) bacteria were observed. A pronounced effect was demonstrated by the sea buckthorn powders on the tested bacteria, mainly showing activity on the Gram-positive strains *S. aureus* ATCC 25923 and *B. cereus* ATCC 6633. Rosehip preparations have a more moderate effect on the tested Gram-positive microorganisms, and chokeberry and hawthorn have a lower antibacterial activity value against these microorganisms. Sea buckthorn powders were more active on *E. coli* ATCC 25922, *Klebsiella pneumonia*e ATCC 13883, and chokeberry and hawthorn demonstrated lower activity.

The antibacterial effect of grape marc, rosehip and sea buckthorn powders was determined after a period of two years. The degree of inhibition of these preparations on Gram-negative and Gram-positive bacteria was practically unchanged over time. The activity of sea buckthorn over time was not significantly modified, and a higher activity was determined on Gram-negative bacteria. It was found that sea buckthorn, rosehip and pomace powders are significantly effective against the growth of *Listeria monocytogenes* ATCC 19118. Water-soluble and fat-soluble extracts from plant powders (sea buckthorn, rosehip, grape pomace) demonstrated marked antibacterial activity on the *L. monocytogenes* EGDe strain. The results obtained by the method of successive double dilutions showed that Gram-positive bacteria (*S. aureus, B. cereus, L. monocytogenes*) are more sensitive than Gram-negative bacteria (*E. coli, S. Abony, K. pneumoniae*). Following the tests carried out, it was found that the powders from sea buckthorn and sea buckthorn meal achieve pronounced MICs against all pathogenic microorganisms investigated, mainly against Gram-positive microorganisms. Rosehip powders possess very high antimicrobial activity against *S. aureus* ATCC 25923 and *B. subtilis* ATCC 6633. Gram-negative bacteria are less sensitive to the effect of plant powders.

Keywords: berry extracts, berry powders, microbiostatic effect, Gram-positive & Gram-negative strains

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OL17

Acaricidal efficacy of cobalt complex in beekeeping

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In recent years, the issue of protecting bee colonies from the parasitic mite *Varroa destructor* has become one of the most pressing challenges in beekeeping. This external parasite mite feeds and reproduces on *Apis cerana* and *Apis mellifera*, causing significant losses in honeybee colonies, and reducing their health and productivity. New methods are being developed to combat this parasite, among which chemical compounds with high efficacy and low toxicity hold particular importance [1-4]. However, currently available treatments do not always demonstrate sufficient activity.

This study conducted biological experiments with the complexes $[Co(C_4H_9N_3S)_3](NO_3)_3]$ aimed at determining its activity against *V. destructor.* Initially, the maximum permissible dose for safe application was established through toxicological testing on *Daphnia magna*. The toxicity analysis revealed that the LC_{50} for the cobalt complex is 56µM after 24 hours and 21µM after 48 hours of incubation. Morphological analysis of the parasites *V. destructor* was performed at different stages of their life cycle to identify the species and assess their response to the tested cobalt complex. Effectiveness was evaluated using concentrations of 1, 10, and 100 µM, and it was found that the LC_{50} for the cobalt complex is 3µM.

Furthermore, field studies on bee colonies in apiaries demonstrated promising results, confirming the high acaricidal activity of the cobalt complex under *in vitro* conditions.

These findings suggest that using the tested compound in bee feed could serve as an effective and safe method for reducing parasite populations. This approach can help improve the health and productivity of bee colonies and significantly reduce economic losses in beekeeping.

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References

1. Garbuz, O.; Gudumac, V.; Toderaș, I.; Gulea, A. Antioxidant Properties of Synthetic Compounds and Natural Products. Action Mechanisms. Monograph; CEP USM: Chișinău, Moldova, 2023; ISBN 978-9975-62-516-6.
2. Garbuz, O.; Toderas, I.; Gulea, A. Biological Properties of Some Synthetic and Natural Compounds. Correlation of Anticancer and Antioxidant Activities. Monograph. = Proprietăţile Biologice ale Unor Compuşi Sintetici şi Naturali. Corelarea Activităţii Anticancer şi Antioxidante. Monografie; Tipografia Centrală: Chișinău, Moldova, 2024; 271p, ISBN 978-5-88554-387-3.
3. Garbuz, O.; Ceban, E.; Istrati, D.; Railean, N.; Toderas, I.; Gulea, A. Thiosemicarbazone-Based Compounds: Cancer Cell Inhibitors with Antioxidant Properties. *Molecules* 2025, *30*, 2077. https://doi.org/10.3390/molecules30092077
4. Garbuz, O.; Graur, V.; Tsapkov, V.; Railean, N.; Toderas, I.; Gulea, A. Chloride tris[*N*-(prop-2-en-1-yl)hydrazinecarbothioamide]-cobalt(III) as a stimulator of the total antioxidant status of *Apis Mellifera*., in Proceedings of the 2nd International Electronic Conference on Antioxidants, 7–9 April 2025, MDPI: Basel, Switzerland.

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OL18

The use of bioprotective yeasts to reduce sulfite consumption in winemaking

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The use of chemical preservatives in food products is a source of controversy, and oenology is no exception, especially regarding the use of sulfur dioxide (SO_2). Faced with societal expectations and increasingly strict legislative requirements, winemakers are increasingly inclined to produce wines with reduced or even no sulfite content. However, their total elimination remains a risky decision, with insufficiently studied consequences on the fermentation processes and the chemical and sensory characteristics of wines. In this context, the use of non-Saccharomyces yeasts as bioprotective agents is considered a viable alternative to the classic initial sulfite treatment.

The objective of this study was to apply comparative analysis of the effect of applying bioprotection to reduce sulfur dioxide content in three distinct wine-growing regions of the Republic of Moldova: Codru IGP Zone, Ștefan Vodă IGP Zone and Valul lui Traian Zone. Each region was represented by a different producer, producing a red wine from locally harvested grapes, subjected to the same bioprotection winemaking protocol.

Bioprotection was ensured by using a commercial formulation of active dry yeast – Primaflora® VR BIO (Oenolia group) – a mixture of Metschnikowia pulcherrima and Saccharomyces cerevisiae, with a concentration of 10^{10} CFU/g. Inoculation was performed on fresh, destemmed must, in the pre-fermentation phases, at a dose of 7 g/hL, adapted to the sanitary quality of the grapes. In parallel, in the control methods, the action of these yeasts was compared with batches without the addition of SO_2. The main purpose of this process is to ecologically occupy the available microbial niche, thus limiting the development of spoilage microorganisms (including acetic acid bacteria) and the risk of early oxidation.

Each batch was fermented with Saccharomyces cerevisiae FERMOL® Premier Cru (AEB group) – a strain intended for red wines, recognized for enhancing aromatic finesse and tannic structure.

Finally, the sensory differences between the different methods of alcoholic fermentation on wines at different stages will continue the research initiated.

Keywords: wines, bioprotection, sulfur dioxide, spoilage microorganisms, sensory quality.

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OL19

Improvement of the water quality of the Bâc river using the example of intensifying the process of purifying ammonia nitrogen in Chișinău MWWTP water

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One of the problems of the surface aquatic environment is the lack of a technological infrastructure for the quality purification of wastewater, which causes pollution of rivers and lakes. One of the most polluted rivers in the Republic of Moldova is the Bâc River. The springs of this river begin in the forest area, the "Plaiul Fagului" reservation, but are blocked with concrete structures, and their water is pumped to the village of Temeleuți, Călărași, from where the waste water flows into the river. The river pollution continues in the same way until Chisinau. Starting from the discharge point into the Bâc River of the waters from the Chisinau Municipal Biological Wastewater Treatment Plant (MWWTP), which exceeded the discharge MAC in 2011-2012 by about 25 times for ammonium and about 4 times for the BOD_5 index, the Bâc River is transformed into an atrophic aquatic body. Dissolved oxygen decreases from the size of a few units (mg O/L) upstream of the discharge of waters from the MWWTP to very low levels and often even zero. In the 1990s, the procedure for pumping activated sludge (AS) into the primary sedimentator was implemented, this being imposed by the condition of no longer being discharged into the waters of the Bâc River. These transformations had a beneficial impact on the water purification process. The aerobic-anaerobic coagulation process created conditions to accumulate in the newly formed organic sediments the majority quantities of organic cationic substances (biologically active substances, surface active substances, colorants, etc.). In recent years, the aeration systems have been modernized. Thus, the oxidation/consumption process of organic carbon and ammonium has advanced in efficiency. During the current summer period, the ammonium concentration in the effluent reachesvalues of over 5 CMA. The improvement of the quality of the discharge water in the effluent (Bâc River) leaves much to be desired. In order to develop the efficiency of organic carbon consumption and especially of ammoniacal and nitrite nitrogen oxidation, laboratory simulations were carried out with water from the Bâc River, the Chișinău MWWTP and the addition of calcium carbonate and expanded ceramics. Using this type of models, simple ISO methods easily combined with spectroscopic ones are applied. Tests in water samples demonstrated an acceleration of the oxidation of both ammonium and nitrite. The reduction of both regulatory and competing processes implies an improvement in the technological purification process. The reorientation of organic species with different charges creates conditions for improving the purification process. It would seem that this combination of the effect of the two additions contributes to a better acceleration of the purification processes. Previously, however, studies have been conducted on the application of these additions for the simultaneous stimulation of the purification process. It has been shown that the impact of expanded ceramics in the presence of calcium carbonate is lower. For the future, an appropriate succession will be found to achieve sustained full efficiency.

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OL20

The study of groundwater and surface water interaction using geochemical and isotope composition

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Republic of Moldova faces a high risk of climate change impact on water resources. The key hydrologic parameters, such as surface water streamflow, evaporation, snow storage, and soil moisture are highly sensitive to climatic variations. The small changes in air temperature and precipitation can affect surface and groundwater recharge and overall water availability. Understanding of water cycle can provide information for integrated water management in the condition of water scarcity. The important point is the evaluation of the interaction between precipitation surface water and groundwaters. Environmental tracer methods are useful for the investigation of the groundwater recharge and groundwater quality. The most frequently used tracers for the groundwater recharge are stable isotopes of water: oxygen ($\delta^{18}O$) and hydrogen ($\delta^{2}H$). Tritium (^{3}H) is used to estimate the approximate meaning groundwater age. The aim of this study is to evaluate stable isotope composition of principal groundwater aquifers, rivers and precipitation for the understanding of the interaction between them and the study of groundwater recharge capacity. The stable isotope composition in precipitation was analyzed from five GNIP stations (**G**lobel **N**etwork for **I**sotope in **P**recipitation). Two hydrology stations at principal rivers Nistru and Prut were established also for stable isotope analysis and seven principal aquifers were studied: 111 sampling sites (37 springs and 74 wells). The period of the investigation is 2020 – 2024 years. Geochemical composition and stable isotopes of oxygen ($\delta^{18}O$) and hydrogen ($\delta^{2}H$) were studied in the Isotope Hydrology Laboratory of Institute of Chemistry of Moldavian State University using modern equipment obtained from IAEA by the implementation of the National Technical Cooperation (TC) project in 2020 – 2023 years. The tritium analysis was made in the Hydrology Laboratory of IAEA, The quality of the stable isotope analysis was ensured by participation in the intercomparison laboratory exercises organized by IAAE. The comparison of the obtained data with GMWL (**G**lobal **M**eteoric **W**ater **L**ine) demonstrates the following: the bottom unconfined aquifers showed a relative heavier isotope composition of oxygen ($\delta^{18}O$) and hydrogen ($\delta^{2}H$) with deep confined aquifers and evaporation effect; the deep confined aquifers have a lighter isotopic composition and a close regularity in the ratio of stable isotopes of oxygen ($\delta^{18}O$) and hydrogen ($\delta^{2}H$) to GMWL; the Tritium content showed a different age interval from tens to thousand years for studied aquifers. The conceptual hydrogeological model in Republic of Moldova is confirmed by the obtained results included the following: major aquifers interact with each other and with surface waters and should be considered as a single aquifer system; the main factors in the formation of groundwater reserves are the recharge by atmospheric precipitation and the interaction of aquifers with each other and with surface waters; groundwater recharge is determined by vertical infiltration and depends on the lithology and the rock fracturing. The technology of the isotope analysis can provide a better understanding of the groundwater recharge capacity. This investigation was made under support from IAEA by national TC project MOL7001 and regional TC project RER7013.

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OL21

Current concepts on the therapeutic potential of kaempferol-loaded bionanocomposites in corneal regeneration

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Corneal diseases represent a significant global public health issue, ranking second as a cause of blindness after cataracts. Recent epidemiological data estimate that approximately 5.5 million people are affected worldwide [7]. In the context of the need for effective and affordable treatments, recent research has focused on the use of natural compounds, such as flavonoids, which act on multiple mechanisms involved in corneal pathology [3]. Kaempferol, a flavonoid with antioxidant properties, has been highlighted for its low cytotoxicity, anti-inflammatory effects, inhibition of angiogenesis, and suppression of vascular smooth muscle cell migration [2]. Moreover, its ability to induce apoptosis in endothelial cells and reduce the expression of vascular endothelial growth factors (VEGFR-2) has been demonstrated, suggesting potential inhibitory effects on corneal neovascularization [4].

However, direct ocular administration is limited by anatomical barriers and reduced bioavailability [5]. In this context, nanomedicine offers safe, minimally invasive, and cost-effective therapeutic strategies [6]. The use of bionanocomposites loaded with nanoparticles, such as ZnO, Se, Ag, and kaempferol, can serve as promising platforms for controlled release, reducing irritation associated with foreign bodies and allowing for decreased frequency of administration. In addition, the use of nanoparticles may provide further benefits, including the reduction of oxidative stress, antimicrobial effects, improved bioavailability, and enhanced therapeutic efficacy [1].

To overcome these limitations, studies are needed to develop bionanocomposites capable of incorporating kaempferol, enabling controlled delivery, protecting the active compound, and increasing bioavailability at the corneal level.

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References

1. Bachu, R. D., Chowdhury, P., Al-Saedi, Z. H. F., Karla, P. K., & Boddu, S. H. S. (2018). Ocular drug delivery barriers-Role of nanocarriers in the treatment of anterior segment ocular diseases. Pharmaceutics, 10, 28.
2. Chen, A. Y., & Chen, Y. C. (2013). A review of the dietary flavonoid, kaempferol on human health and cancer chemoprevention. Food Chemistry, 138, 2099–2107.
3. Feng, J., & Zhang, Y. (2023). The potential benefits of polyphenols for corneal diseases. Biomedicine & Pharmacotherapy, 169, 115862.
4. Liang, F., Han, Y., Gao, H., Xin, S., Chen, S., Wang, N., Qin, W., Zhong, H., Lin, S., Yao, X., et al. (2015). Kaempferol identified by zebrafish assay and fine fractionations strategy from Dysosma versipellis inhibits angiogenesis through VEGF and FGF pathways. Scientific Reports, 5, 14468.
5. Patel, A., Cholkar, K., Agrahari, V., & Mitra, A. K. (2013). Ocular drug delivery systems: An overview. World Journal of Pharmacology, 2, 47–64.
6. Tsai, C. H., Wang, P. Y., Lin, I. C., Huang, H., Liu, G. S., & Tseng, C. L. (2018). Ocular drug delivery: Role of degradable polymeric nanocarriers for ophthalmic application. International Journal of Molecular Sciences, 19, 2830.
7. Wang, E. Y., Kong, X., Wolle, M., Gasquet, N., Ssekasanvu, J., Mariotti, S. P., Bourne, R., Taylor, H., Resnikoff, S., & West, S. (2023). Global trends in blindness and vision impairment resulting from corneal opacity 1984–2020: A meta-analysis. Ophthalmology, 130(8), 863–871.

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OL22

Evaluation of total flavonoid content in *Aronia melanocarpa* (Michx.) Elliot

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Introduction: *Aronia melanocarpa* (Michx.) Elliot is a plant valued for its health-promoting properties, mainly attributed to its rich content of phenolic compounds, including anthocyanins, phenolic acids, tannins, vitamins, minerals, and especially flavonoids [1].
Aim of the study: To determine the total flavonoid content (TFC) in the fruits and non-edible parts of *A. melanocarpa* cultivars *(*Alexandrina and Nero).
Materials and Methods: Plant material was collected from the Scientific Practical Center in the Field of Medicinal Plants and from the "Alexandru Ciubotaru" National Botanical Garden, Republic of Moldova. TFC was spectrophotometrically determined by the aluminum chloride complexation method.
Results: The TFC of fruits and non-edible parts of *A. melanocarpa* ranged from 1.59 mg QE/g to 6.24 mg QE/g. The highest content was found in the leaves of the Alexandrina cultivar, while the lowest was observed in the three-year-old twigs of the Nero cultivar. In Nero samples, TFC ranged from 1.59 mg QE/g (twigs) to 6.09 mg QE/g (leaves). For Alexandrina, TFC ranged from 1.67 mg QE/g (twigs) to 6.24 mg QE/g (leaves).
Conclusions: In both cultivars, the leaves exhibited the highest flavonoid content, while the three-year-old twigs contained the lowest. These findings suggest that *A. melanocarpa* leaves represent a valuable source of flavonoids, making them of particular interest for research in botany, medicine, and pharmacy.
Key words: *A. melanocarpa*, total flavonoid content, fruits, non-edible parts.
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References

1. Frumuzachi O., Rohn S., Mocan A. Fermented black chokeberry (*Aronia melanocarpa* (Michx.) Elliott) products – A systematic review on the composition and current scientific evidence of possible health benefits. In: Food Research International, 2024, vol. 196, p. 115094. https://doi.org/10.1016/j.foodres.2024.115094

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OL23

FTIR and nano-FTIR spectroscopic insights into the photochemical stability of silsesquioxane hybrid coatings on archaeological ceramics

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The study investigates the chemical and structural evolution of silsesquioxane-based hybrid coatings applied to Neolithic ceramic artifacts from Cucuteni, subjected to accelerated UV aging [1]. A particular emphasis was placed on Fourier transform infrared (FTIR) and nano-FTIR spectroscopy to elucidate the molecular mechanisms underlying the degradation and photooxidation processes. FTIR spectra revealed gradual changes in the intensity and position of the characteristic bands attributed to Si-O-Si, Si-C and C-H stretching vibrations, indicating the partial cleavage of organic groups and the reorganization of the silsesquioxane network under UV irradiation. Second derivative and curve fitting analyses allowed the quantitative assessment of the crosslinking density and the formation of hydroxyl groups, correlating with the surface hydrophilicity. Complementary nano-FTIR mapping provided spatially resolved chemical information at the nanoscale, revealing heterogeneities in the silsesquioxane matrix and localized oxidation phenomena at the coating-substrate interface. The combined FTIR/nano-FTIR approach allowed the identification of subtle chemical changes that precede macroscopic degradation, highlighting the critical role of silsesquioxane architecture in ensuring long-term photostability. These results demonstrate the potential of advanced infrared microspectroscopy as powerful diagnostic tools for assessing the durability and compatibility of protective coatings designed for the conservation of cultural heritage ceramics.

References

2. Oancea, A.V., Bodi, G., Cernescu, A. *et al.* Protective coatings for ceramic artefacts exposed to UV ageing. *npj Mater Degrad* **7**, 21 (2023). https://doi.org/10.1038/s41529-023-00343-8

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POSTER PRESENTATIONS

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PP1.1

Antimicrobial activity of iron(III) complexes incorporating Schiff base ligands

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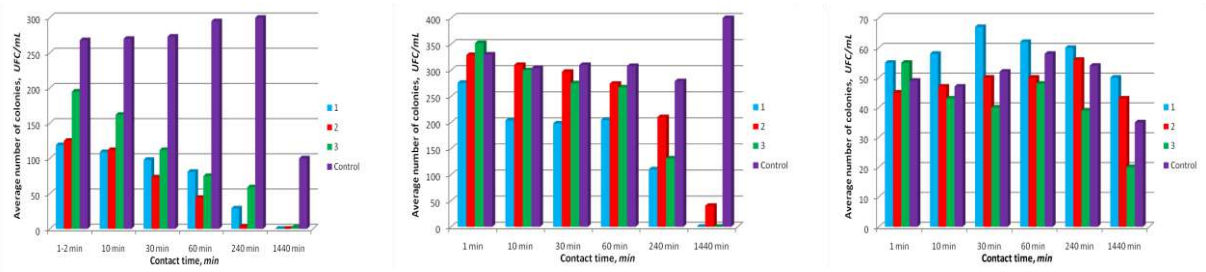
Staphylococcus aureus and *Escherichia coli* are among the primary pathogenic bacteria responsible for both community-acquired and hospital-acquired bacteremia. Among fungal pathogens, *Candida albicans* is recognized as the most common cause of fungal infections in humans. The recent studies have shown that substances with bacteriostatic and bactericidal properties can significantly influence the synthesis and release of antioxidant enzymes in microbial cells.

To evaluate potential antimicrobial activity, three iron(III) coordination compounds $[Fe(H_2L^1)(H_2O)_2](ClO_4)_3{\cdot}2.5H_2O$ (**1**), $[Fe(H_2L^2)(H_2O)_2](ClO_4)_3{\cdot}H_2O$ (**2**) and $[Fe(H_2L^3)(H_2O)_{1.5}(CH_3OH)_{0.5}](ClO_4)_3{\cdot}1.75H_2O$ (**3**) were tested for their bactericidal and bacteriostatic effects [1, 2]. The ligands used were H_2L^1 = 2,6-diacetylpyridine bis(picolinoylhydrazone), H_2L^2 = 2,6-diacetylpyridine bis(nicotinoylhydrazone) and H_2L^3 = 2,6-diacetylpyridine bis(isonicotinoylhydrazone). The antimicrobial activity was assessed against the bacterial strains *Escherichia coli* and *Staphylococcus aureus*, as well as the yeast-like fungus *Candida albicans*.



(a) *(b)* *(c)*

Figure. Colony-forming units of *E. coli (a), S. aureus (b), C. albicans (c)* after exposure to complex **1** (blue), **2** (red), **3** (green) and control, without treatment (violet)

For complexes **1-3**, the bactericidal effect was observed after 1-2 minutes of contact, when a significant decrease of the number of *E. coli* and *S. aureus* colonies compared to the control sample was observed (Figure, *a* and *b*). In the case of gram-negative bacteria *C. albicans*, the compounds showed better activity, thus for complex **1**, the bactericidal effect was observed after 30 minutes of contact, for compound **2** - after 240 minutes, and for compound **3** - after 1-2 min, when a significant decrease of the number of *C. albicans* colonies compared to the control sample was observed (Figure, *c*).

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References

1. Danilescu, O., Bulhac, I., Bourosh, P.N., Croitor, L. Polyhedron, 2022, 215, 115679. https://doi.org/10.1016/j.poly.2022.115679
2. Danilescu, O.; Bourosh, P.; Bulhac, I.; Kulikova, O.; Cocu, M.; Chumakov, Yu. CrystEngComm., 2025, 27, 3006 - 3017. https://doi.org/10.1039/D5CE00125K

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PP1.2

Synthesis and characterization of 3,4-dihydropyrimidin-2-ones with biological potential, in the presence of organic catalysts

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Abstract. In recent years, there has been a significant increase in the number of publications focused on the chemistry of 3,4-dihydropyrimidin-2-ones synthesized via the Biginelli three-component condensation reaction.

This growing interest is attributed not only to the straightforward synthetic accessibility of these compounds but also to their broad spectrum of pharmacological activities, including analgesic, antibacterial, and antihypertensive effects, among others. These properties make further research in this class of compounds particularly promising [1].

3,4-Dihydropyrimidin-2(1*H*)-ones are known to act as antihypertensive agents, α1-adrenergic receptor antagonists, and neuropeptide antagonists. Moreover, they are found as core structural motifs in various marine alkaloids that exhibit potent anti-HIV activity.

Introduction. The scope of application of 3,4-dihydropyrimidin-2-ones was considerably expanded with the synthesis of an important derivative – 4-(3-hydroxyphenyl)-pyrimidin-2-one, known as oxymonastrol. This compound stood out with a completely new mechanism of antitumor action, due to its specific influence on the process of cell division (mitosis).

Unlike its analogue monastrol, in which the oxygen atom is replaced by a sulfur atom, oxymonastrol exhibits a more selective and longer-lasting action, being cytotoxic only at the highest concentrations used, without affecting cell proliferation or viability. This property has essential therapeutic significance.

These properties are also valid for racemic oxymonastrol [2].

The significant biological role of oxymonastrol and its derivatives has attracted particular interest in its synthesis, achieved by a one-pot reaction with three components – ethyl acetoacetate, urea and 3-hydroxybenzaldehyde. This method avoids the generation of waste associated with multi-step purifications and minimizes residues.

In addition, the obtained adducts include in their structure almost all atoms coming from the reactants, reflecting the so-called atomic efficiency, and water is the only by-product of the reaction.

From the point of view of environmental requirements for protecting the ecosystem in the modern world, it is proposed to use β-cyclodextrin and pectin with low esterification content as catalysts.

Conclusions. Availability of the reagents used, possibility of reuse, simplicity of the synthesis method and the method of purification of the final product by crystallization, compliance with the linear relationship between the theoretical principles of green chemistry and practical application experience, characteristics that allow for the greatest possible approximation to ecological catalytic conditions.

References

1. Mayer T.U., Kapoor T. M., Haggarty S. J., King R. W., Schreiber S. L, Mitchison T. J. Small molecule inhibitor of mitotic spindle bipolarity identified in a phenotype-based screen. Science, 1999, 286, 971 p.
2. Culacov I., Talipov S., Suligav Z., Seilhanov T. Synthesis, structure and antiradical activity of new derivatives of methano[1,3]thiazolo-[2,3-d][1,3,5] benzoxadiazocin. Chemistry of heterocyclic compounds, 2014, 10, pp. 1604—1613.

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PP1.3

Synthesis of new biologically active homodrimane sesquiterpenoids with phenothiazine fragment

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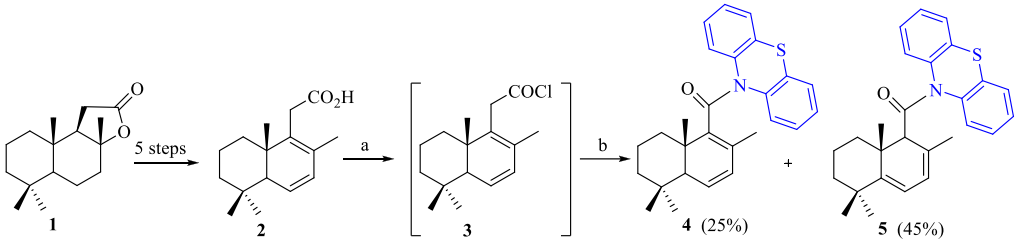
In recent years, the rapid spread of microbial infections has become a major global health issue, driving the search for new antimicrobial compounds. Natural products are a key source of such agents due to their biocompatibility, selective activity, and low toxicity. Terpenes, especially those with a homodrimane sesquiterpene skeleton, are natural compounds with a wide range of pharmaceutical and biological activities. Previously, it has been reported that molecular terpeno-heterocyclic hybrids possessing oxadiazole, thiadiazole, benzothiazole, benzimidazole and other heterocyclic units have shown good antifungal and antibacterial activities [1-3].

As starting material for the synthesis of the title compounds was 11-homodrim-6(7),8(9)-dien-12-oic acid **2**, prepared in five steps from commercially available (+)-sclareolide **1** [4]. The final homodrimane phenothiazine hybrids **4** and **5** were obtained by acylation of phenothiazine with the acyl chloride **3** (generated *in situ* from acid **2**) under the conditions described in the Scheme. The structures of the synthetized compounds have been established using modern spectral methods of analysis (ATR-FTIR, ^{1}H, ^{13}C and ^{15}N NMR).



Scheme. ***a****. $(COCl)_2$, C_6H_6, r.t., 1h, Δ, 1h;* ***b****. Phenothiazine, CH_2Cl_2, r.t., 24h.*

The antifungal and antibacterial activities of the title compounds were assessed by performing "*in vitro*" tests against five species of fungi (*Aspergillus niger*, *Fusarium*, *Penicillium chrysogenum*, *P. frequentans* and *Alternaria alternata*) and two species of bacteria (*Pseudomonas aeruginosa* and *Bacillus* sp.). Compound **5** exhibited the highest antifungal activity, with a MIC of 0.05 µg/mL, being 6 times higher than that of the reference compound Caspofungin (MIC = 0.32 µg/mL). Additionally, it showed extremely high antibacterial activity, with a MIC of 0.064 µg/mL, being 62 times higher than that of the reference compound Kanamycin (MIC = 2 µg/mL). Compound **4** had no inhibitory effect against the tested fungi and bacteria.

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References

1. Lungu, L., Ciocarlan A., Smigon C., Ozer I., Shova S., Gutu I., Vornicu N., Mangalagiu I., D'Ambrosio M., Aricu A. Chem. Heterocycl. Compd., 2020, 56, 578–585. DOI: https://doi.org/10.1007/s10593-020-02703-7
2. Lungu, L., Cucicova, C., Blaja, S., Ciocarlan, A., Dragalin, I., Barba, A., Kulciţki, V., Vornicu, V., Geana, E., Mangalagiu, I.I., Aricu, A. Molecules, 2023, 3(28), 933-946. DOI: https://doi.org/10.3390/molecules28030933
3. Lungu, L., Cucicova, C., Blaja, S., Ciocarlan, A., Dragalin, I., Vornicu, N., Geana, E., Mangalagiu, I.I., Aricu, A. Molecules, 2022, 27, 5082-5096. DOI: https://doi.org/10.3390/molecules27165082
4. Duca, Gh., Aricu, A., Lungu, L., Tenu, N., Ciocarlan, A., Gutu, Y., Dragalin, I., Barba, A. Chem. J. Mold., 2018, 13(1), 69-73. DOI: http://dx.doi.org/10.19261/cjm.2017.458

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PP1.4

Synthesis of low molecular weight prenylated acylguanidine derivatives as prospective antimicrobial agents

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In the contemporary world, one of the critical vulnerabilities in maintaining and preserving public health is the urgent need for the use of sustainable antimicrobial agents. This trend is directly associated with the emergence of multidrug-resistant bacteria, which can be naturally explained by their rapid adaptation to the antimicrobial agents applied.

One of the approaches to addressing this dilemma involves the use of natural metabolites [1] or hemisynthetic analogues incorporating a guanidine-containing moiety [2]. The uniqueness of this unit lies in its unusual nature. On one hand, it can be considered a nitrogen-containing analogue of a carboxylic acid, whose basicity is determined by the structural features of the surrounding radicals. On the other hand, it possesses the ability to form strong hydrogen bonds with proteins or other target compounds, in addition to facilitating cation-anion interactions, which constitute the basis of molecular recognition mechanisms in physiological environments. Therefore, the ability of the guanidine fragment to act as either a base or an acid explains its presence in the design of many therapeutic molecules [3].

Continuing our previous research on the synthesis of guanidine-containing antimicrobial compounds [4], a series of new low-molecular acylguanidines **1-4** (*figure 1*) was obtained. The starting material for the syntheses was the commercially available labdane diol sclareol, which, following oxidative degradation reactions, yielded a series of the corresponding acids. The interaction between the "activated" forms of these acids and a mixture of guanidine-base smoothly led to the formation of the desired guanidines **1-4**. The structures and stereochemistry of the new compounds were established based on their spectral data.

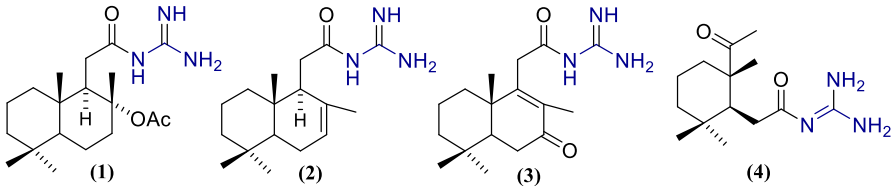

Figure 1. Synthesized prenylated acylguanidines.

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References

1. Berlinck, R. G. S., Bernardi, D. I., Fill, T., Fernandes, A. A. G., Jurberg, I. D. Natural Product Reports, 2021, 38, 586-667. DOI: https://doi.org/10.1039/D0NP00051E
2. Saczewski, F., Balewski, L. Expert Opinion on Therapeutic Patents, 2013, 23(8), 965-995. DOI: https://doi.org/10.1517/13543776.2013.788645
3. Kim, S.-H., Semenya, D., Castagnolo, D. European Journal of Medicinal Chemistry, 2021, 216, 113293. DOI: https://doi.org/10.1016/j.ejmech.2021.113293
4. Grinco, M., Morarescu, O., Lembo, F., Ungur, N., Turco, L., Coretti, L., Carbone, M., Celentano, C., Ciavatta, M. L., Mollo, E., Kulcitki, V., Buommino, E. European Journal of Medicinal Chemistry, 2024, 264, p. 115981. DOI: https://doi.org/10.1016/j.ejmech.2023.115981

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PP1.5

Tuning the adsorptive properties of zinc-based MOFs through controlled synthesis conditions

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Metal–organic frameworks (MOFs), a class of coordination polymers, have become a central topic in modern scientific investigation and technological development. Their remarkable capacity to interact with neutral molecules, especially in the contexts of gas capture and separation processes, has attracted widespread interest in the last two decades. Structurally, MOFs consist of inorganic clusters connected by rigid organic ligands, forming extended networks. This architectural design imparts them with multifunctionality, enabling uses in areas such as gas adsorption, molecular sensing, targeted drug transport, and biomedical applications. Due to their exceptional porosity, large internal surface area, and tunable characteristics, MOFs have drawn intense attention from researchers focused on advanced material synthesis.

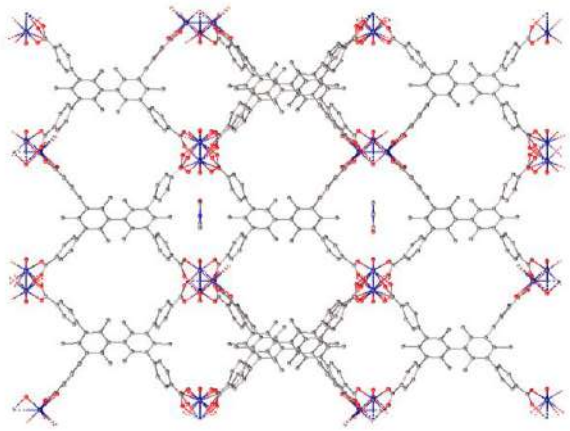

Fig. 1. View of 3D MOF **1** along axis *a*

In this study, we report the synthesis, structural characterization, and properties of two novel zinc-based MOFs, constructed using 3,3',5,5'-tetrakis(4-carboxyphenyl)-2,2',4,4',6,6'-hexamethyl-1,1'-biphenyl (**H_4L**) as the organic linker. The MOFs were synthesized via solvothermal reactions between H_4L and $Zn(NO_3)_2$ under different conditions. Notably, slight changes in the solvent system led to the formation of distinct frameworks: polymer **$[Zn_4L_2(H_2O)_3]$** (**1**) was obtained from a DMF/H_2O mixture, whereas compound **$[Zn_2L]$** (**2**) crystallized from pure DMF. Single-crystal X-ray diffraction analysis revealed that both compounds possess three-dimensional coordination networks formed by zinc ions acting as nodes and L^{4-} ligands serving as polydentate linkers. Compound **1** crystallizes in the monoclinic space group *Pnnm*, while compound **2** in *P-1*. Both MOFs demonstrate thermal stability up to 400 °C and exhibit permanent porosity. However, due to their structural differences, they display distinct BET surface areas: 250 m^2/g for **1** and 48 m^2/g for **2**.

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PP1.6

Quinoline derivatives with potential antimicrobial activity

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Azaheterocycles derivatives, quinoline including, are invaluable scaffolds from pharmacological point of view, having a large variety of biological activities such as antimicrobial (antibacterial and antifungal, antiplasmodial, antitubercular, etc), anticancer, anti-inflammatory, antidepressant, analgesic, anti-Alzheimer's, antihypertensive, etc. [1-9].

As part of our continuous efforts in the field of azaheterocyclic derivatives, we present herein some core results obtained by our group in the field of quinoline with antimicrobial activity [10-14]. The quinoline derivatives were synthesized by efficient and direct reaction pathway, by using conventional thermal heating and eco-friendly methods (by microwave and ultrasound irradiation). The antimicrobial activity of the quinoline derivatives was determined, some of the compounds having a very good antimicrobial activity. Some of the obtained compounds are promising leading drug candidates.

References

1. Silverman, R.B.; Holladay, M.W. The organic chemistry of drug design and drug action, 3rd Edition; Academic Press, London, 2014; ISBN: 9780123820303.
2. Diaconu, D.; Savu, M.; Ciobannu, C.; Mangalagiu, V.; Mangalagiu, I.I. Bioorg. Med. Chem. 2025, 119, 118069.
3. Amariucai-Mantu, D.; Antoci, V.; Sardaru, M. C.; Al Matarneh, C. M.; Mangalagiu, I.I.; Danac, R. Phys. Sci. Rev. 2022, 8(9), 2583-2645.
4. Lungu, C.N.; Bratanovici, B.I.; Grigore, M.M.; Antoci, V.; Mangalagiu I.I. Curr. Med. Chem. 2020, 27(1), 154-169.
5. Antoci, V.; Oniciuc, L.; Amariucai-Mantu, D.; Moldoveanu, C.; Mangalagiu, V.; Amarandei, A.M.; Lungu, C.N.; Dunca, S.; Mangalagiu, I.I.; Zbancioc, G. Pharmaceuticals 2021, 14, 335.
6. Popovici L., Amarandei R.M., Mangalagiu I.I., Mangalagiu V., Danac, R. J. Enzyme Inhib. Med. Chem. 2019, 34, 230-243.
7. Olaru A., Vasilache V., Danac R., Mangalagiu I.I. J. Enzyme Inhib. Med. Chem. 2017, 32, 1291-1298.
8. Luca, M.C, Tura, V; Mangalagiu I.I. Med. Hyp. 2010, 75, 627-629.
9. Zbancioc G., Bejan, V., Risca M., Moldoveanu, C., Mangalagiu I.I. Molecules 2009, 14, 403-411.
10. Diaconu, D.; Mangalagiu, V.; Dunca, S.; Amăriucăi-Mantu, D.; Antoci, V.; Roman, T.; Mangalagiu, I.I. Heliyon 2023, 9, e21518.
11. Diaconu, D.; Antoci, V.; Mangalagiu, V.; Amariucai-Mantu, D.; Mangalagiu, I.I. Sci. Rep. 2022, 12, 16988.
12. Diaconu, D.; Amariuci-Mantu, D.; Mangalagiu, V.; Antoci, V.; Zbancioc, Ghe.; Mangalagiu, I.I. RSC Adv. 2021, 11, 38297–38301.
13. Al-Matarneh, M.C.; Amarandi, R.M.; Mangalagiu, I.I.; Danac, R. Molecules 2021, 26, 2066.
14. Diaconu, D.; Mangalagiu, V.; Amariucai-Mantu, D.; Antoci, V.; Giuroiu, C.L.; Mangalagiu, I.I. Molecules 2020, 25, 2946.

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PP1.7

Quantitative thermodynamic modeling of drug precipitation-dissolution in cyclodextrin-based multicomponent aqueous systems

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An original thermodynamic methodology has been developed to quantitatively assess drug precipitation phenomena in heterogeneous systems composed of drug, cyclodextrin, and auxiliary agents. For the first time, the concept of the *degree of drug precipitation* has been formally introduced and defined using unique mass balance equations in combination with the Law of Mass Action. By utilizing established thermodynamic data, it becomes possible to determine the distribution of all drug-containing species in both the aqueous and solid phases as functions of pH and chemical composition. The molar fractions of species such as free drug, ionized forms, and binary or ternary complexes are expressed as normalized ratios relative to the total apparent solubility, maintaining internal consistency within the system.

The degree of precipitation is defined as the molar fraction of the drug present in the solid state, expressed as a percentage. This provides a direct and quantitative measure of solubility limitations under specified conditions.

To analyze species distribution across varying chemical environments, a new graphical method called *Diagrams of Heterogeneous Chemical Equilibria* has been introduced. This includes three key stages: (1) thermodynamic evaluation of solid phase stability based on precipitation degree, (2) determination of species molar fractions within the drug stability area, and (3) for systems where only soluble species are present, the molar fractions are calculated using standard methods typically applied in homogeneous equilibrium studies. The developed thermodynamic approach enables accurate modeling of phase behavior, complex formation, and distribution of chemical species in multicomponent aqueous environments.

The proposed framework represents a significant advancement in pharmaceutical thermodynamics, offering both quantitative and visual tools to investigate solubility and precipitation behavior. The approach was successfully applied to ten commercial drugs and can be extended to a broad range of poorly soluble compounds in pharmaceutical, environmental, and materials science research.

Acknowledgments: This work has been carried out within the Research and Innovation Program ”Stimulating excellence in research”, „*The thermodynamic elucidation and prediction of chemical synergism in complex chemical processes*”, 2024-2025, code 20.80012.5007.19SE. A part of the work was carried out within the Institutional Research Program of the State University of Moldova for the period 2024-2027, subprogram “*Advanced Research in Computational and Environmental Chemistry, Identification of Technological Treatment Processes, Formation of Water Quality and Quantity*”, code 010603.

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PP1.8

^{1}H NMR Studies of the interactions of three chromenol derivatives with Drew-Dickerson Dodecamer

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DNA - a crucial macromolecule in biological systems is frequently targeted by pharmaceutical agents. Particularly, studying the DNA-binding properties of antifungal agents is essential for understanding their mechanisms of action and enhancing therapeutic selectivity [1]. NMR spectroscopy is a method o choice for characterizing nucleic acid dynamics [2] and the pursuit of antifungal ligands with strong DNA-targeting potential, guided by NMR analysis, holds great promise for identifying clinically relevant DNA-binding compounds.

This paper showcases three 1*H*-1,2,4-triazole functionalized chromenols **1-3** as novel powerful antifungal agents [3]. Dickerson−Drew dodecamer (DDD) - one of the most studied prototypic B-DNA molecules with a palindromic oligonucleotide sequence has been used [4].

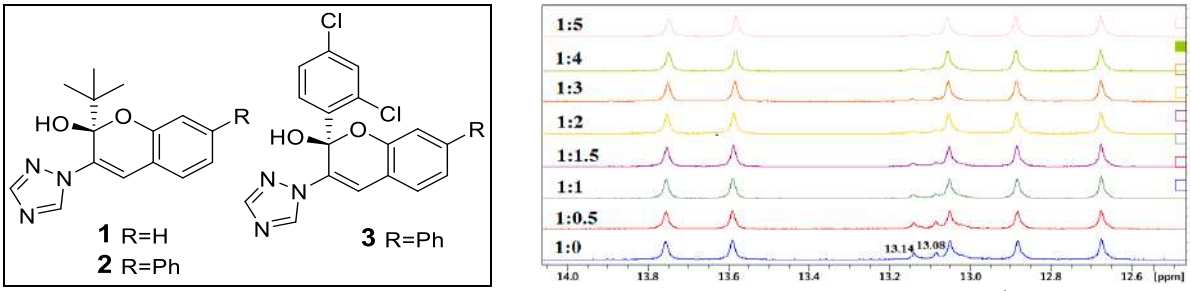

Figure 1. Chemical structures of the used ligands **1-3** [3] and imino- region of the ^{1}H NMR titration spectra of DDD in 10 mM KPi (pH 7.0), 10 % D_2O (25 °C, 600 MHz). For conformity, the DDD-**3** case is illustrated; the DDD-**3** ratio is shown at the left side of the spectra.

The ^{1}H NMR data give evidence about non-recognition of the major homodimeric form of DDD by ligands **1-3**, as both chemical shift and shape of signals for the indicative imino protons do not vary upon titration (Figure 1). Nonetheless, small changes were noticed in spectra characterizing the presence of minor DDD conformer in solutions, attested by small peaks at δ 13.08 and 13.14 ppm. Broadening of these signals upon ^{1}H NMR titrations testifies the occurrence of nonspecific interactions between compounds **1-3** and the minor conformer structures, most likely, a hairpin, of the model DNA.

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References

1. Özkul, M.A. et al. Spectrochim. Acta Part A: Mol. Biomol. Spectrosc., 2025, 341, 126351. https://doi.org/10.1016/j.saa.2025.126351
2. Al-Hashimi, H.M. J. Magn. Reson., 2013, 237, 2013, 191-204. https://doi.org/10.1016/j.jmr.2013.08.014
3. Zveaghintseva, M. et al. Molecules, 2021, 26, 4304. https://doi.org/10.3390/molecules26144304
4. da Rosa, G. et al. Biophys. Rev., 2021, 13, 995-1005. https://doi.org/10.1007/s12551-021-00893-8

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PP1.9

Antiproliferative activity of a dinuclear Cu(II) complex with a cyclized carbohydrazone ligand

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The identification of compounds with antiproliferative activity against the HeLa cell line is of utmost importance, as they represent essential experimental models for understanding and combating cervical cancer - one of the most common forms of cancer among women globally, especially in regions with limited access to screening and treatment.

To evaluate the in vitro antiproliferative potential of the ligand H_4L=1,5-bis(3-methoxy-salicylaldehyde)thiocarbohydrazone and the coordination compound $[Cu_2(H_2Lcycl)(CH_3OH)_2Cl_3]\cdot CH_3OH$ [1] (Figure), where H_2L is cyclized form of the mentioned proligand, they were tested on HeLa cancer cells using the resazurin assay.

In this study, HeLa cells were cultured in Dulbecco's Modified Eagle Medium (DMEM), supplemented with fetal bovine serum and antibiotics, to assess the antiproliferative effect of the newly synthesized compounds.

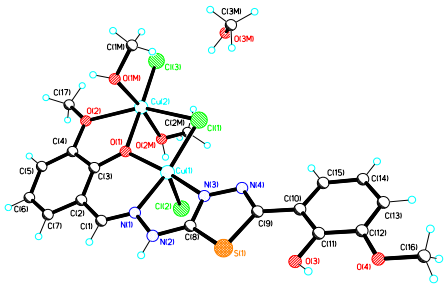

Figure. Molecular structure of the compound $[Cu_2(H_2L_{cicl})(CH_3OH)_2Cl_3]\cdot CH_3OH$.

The proligand (H_4L) has antiproliferative activity against the HeLa cancer cell line $IC_{50} \geq 10$ μg/ml, and the coordinating compound $[Cu_2(H_2L_{cicl})(CH_3OH)_2Cl_3]\cdot CH_3OH$ based on this proligand showed a value of IC_{50} = 10,5±0,1 μg/ml, comparable to that of DOX (doxorubicin) IC_{50} =10,0±0,4 μg/ml, used in medicine.

The IC_{50} value expresses the concentration required for 50% inhibition of cell viability.

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References

1. Talmaci, N., Bourosh, P., Kravtsov, V., Dragancea, D. Dinuclear Cu(II) complex with a novel carbohydrazone Schiff base ligand containing 1,3,4-thiadiazole. The International Conference dedicated to the 55th anniversary from the foundation of the Institute of Chemistry of the Academy of Sciences of Moldova, 28-30 May 2014, Chisinau. Republic of Moldova: USM Institute of Chemistry, 2014, p. 125.

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PP1.10

Quinoline functionalization for the obtaining of biologically useful compounds

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Quinoline is a versatile heterocyclic compound commonly used in medicinal chemistry. Quinoline derivatives exhibit a variety of biological activities, including antibacterial, antifungal, antimalarial and anticarcinogenic properties [1].

The corresponding quinolinium salts were synthesized through the reaction of quinoline or quinoline derivatives with bromoacetone or 1-bromopinacolone. The alkylation reaction occurred via an S_N2-type mechanism, whereby the nucleophilicity of the nitrogen atom in quinoline enabled reaction with the activated halogenated derivative, resulting in the formation of quinolinium salts [2]. The presence of a methyl or tert-butyl group in the side position endows these salts with significant steric and electronic properties that could affect their reactivity in subsequent stages.

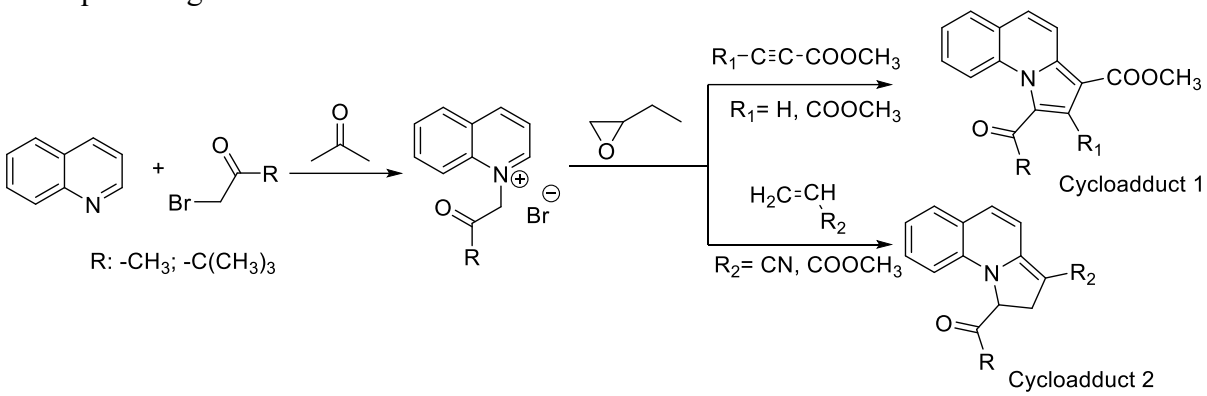

Figure 1. Dipolar [3+2] cycloaddition reactions of quinolinium salts with activated alkenes or alkynes.

These quinolinium salts underwent [3+2] Huisgen-type cycloaddition reactions with activated alkynes [3,4]. These reactions proceeded in a stereospecific manner, without the formation of regioisomers, and produced stable tetracyclic azacyclic derivatives with promising pharmacological potential. This approach yielded useful new functionalised compounds for further exploration in medicinal chemistry.

Acknowledgments: The authors express their gratitude to the RECENT AIR project (grant MySMIS no. 127324) for facilitating access to the laboratory, and to the POSCCE-O 2.2.1 project (SMIS-CSNR 13984-901, no. 257/28.09.2010, CERNESIM) for supporting the NMR experiments.

Keywords: azaheterocycle, quinoline, nucleophilic substitution, medicinal chemistry, cycloadditions.

References

1. Yadav, P., Shah, K., Biorganic Chemistry, 109, 104639, (2021).
2. Marek J, Buchta V, Soukup O, Stodulka P, Cabal J, Ghosh KK, Musilek K, Kuca K., Molecules.,17(6):6386-6394, (2012).
3. Mandal A., Khan, A., Organic & Biomolecular Chemistry, 22, 2339, (2024).
4. Zbancioc, G.; Mangalagiu, I.I.; Moldoveanu, C., Pharmaceuticals, 17, 52, (2024).

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PP1.11

Synthesis, characterization and enzymatic activity enhancement of the heterobimetallic complex $[CaL_3][Co(NCS)_4]$ on *Rhizopus arrhizus* CNMN FD 03

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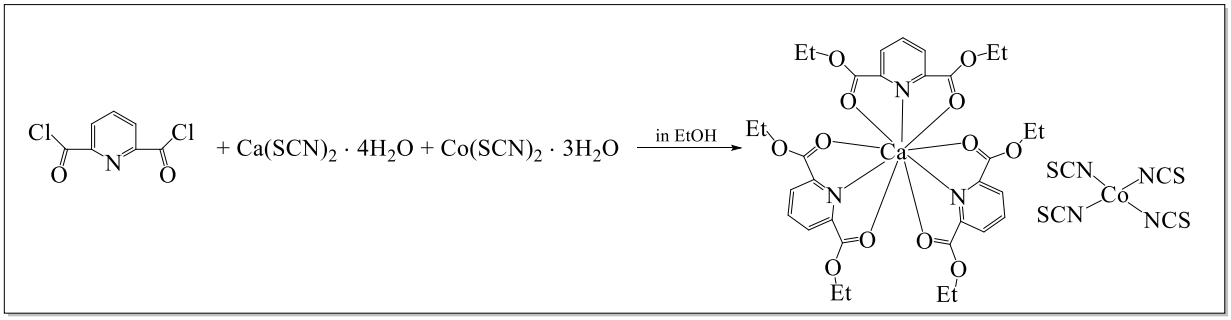
Diethyl pyridine-2,6-dicarboxylate (L) was prepared by refluxing pyridine-2,6-dicarbonyl dichloride in ethanol, and the reactions of L with Ca(II) and cobalt(II) thiocyanates resulted in the formation of a heterobimetallic complex $[CaL_3][Co(NCS)_4]$. The reaction equation proceeded according to the following scheme:



The obtained complex was studied using elemental analysis and IR spectroscopy. The investigated complex is an ionic compound consisting of the complex cation $[CaL_3]^{2+}$ and the complex anion $[Co(NCS)_4]^{2-}$. Additionally, the complex was subjected to microbiological testing on the *Rhizopus arrhizus* CNMN FD 03 micromicete strain. The data with the test results are presented in the table.

Table. The influence of the coordination compound $[CaL_3][Co(NCS)_4]$ on the lipolytic activity of the micromycete *Rhizopus arrhizus* CNMN FD 03

Compound	Conc., mg/L	1st day		2nd day		3rd day	
		Activity, mg/L	%, control*	Activity, mg/L	%, control	Activity, mg/L	%, control
$[CaL_3]$ $[Co(NCS)_4]$	5	41125,0	198,6/137,1	19375,0	64,6	2083,3	9,4
	10	28291,7	136,6/94,3	25000,0	83,3	2083,3	9,4
	15	20125,0	97,2	23750,0	79,2	1259,0	5,7
Control	-	20708,3	100,0	30000,0	100,0	22083,3	100,0

*198,6/137,1 - relative to the day's control/relative to the maximum value of the control from day 2

It is worth noting that metal-complex significantly enhances the accumulation of lipolytic enzymes in the studied strain, with the highest increase in enzymatic activity (98.6% compared to the reference sample on the same day) observed at a concentration of 5 mg/L. The enzymatic activity value recorded in this variant (41,125.0 U/mL) even exceeds the upper level of the control sample from the second day of cultivation, representing a 37.1% increase. When applied at a concentration of 10 mg/L, the compound ensures a 36.6% increase in enzymatic activity compared to the control of the same day, with the activity level being almost equal to the maximum value of the reference sample (94.3%).

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PP1.12

Infrared spectroscopy of human urinary stones in Republic of Moldova

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Urinary lithiasis occupies an important place in the structure of urological diseases with a percentage of 10-40%. Nephrolithiasis has an estimated frequency between 1.0% and 12.0% of the general population causing high disability (approximately 11% of patients with kidney stones). The high rate of invalidation places nephrolithiasis in third place among urological pathologies after neoplasms and urinary infections. Currently, in the Republic of Moldova, there is an increase in the incidence of urolithiasis, which from 2005 to the present has occupied the first place in the structure of diseases in urological clinics, leaving behind inflammatory pathologies and prostate adenoma. The prevalence of urolithiasis is about 10% in the country's population.

Infrared spectroscopy is a modern analytical method for studying the chemical composition of urinary stones. The composition of kidney stones may indicate a possible etiopathogenic mechanism responsible for their formation.

The spectra were recorded on IR Fourier spectrometer Spectrum 100 (Perkin Elmer, USA) using an ATR (Attenuated Total Reflectance) accessory in the range 4000 – 650 cm^{-1}. Urinary stones obtained from patients of the Department of Urology and Surgical Nephrology (Nicolae Testemitanu State University of Medicine and Pharmacy), the Section of Urology (Timofei Mosneaga Republican Clinical Hospital), Novamed Polyvalent Hospital, IMSP SCM "Holy Trinity" of Chisinau of the Republic of Moldova were investigated in 2015 - 2024. Electronic databases of IR spectra of individual substances, atlases of IR spectra, and other reference and scientific literature on IR spectroscopy were used for interpretation.

Thus the method of Fourier Transform (FT) Infrared (IR) Attenuated Total Reflectance (ATR) Spectroscopy was perspective to use for studying the chemical composition of urinary stones. 270 urinary stones (157 men (57.5%) and 113 women (42.5%), aged 18-75 years, the ratio is 1.4 : 1) of patients living in the territory of the Republic of Moldova were examined. The results of stone composition can provide valuable information for the diagnosis, treatment and recurrence prevention of urolithiasis. The most common were oxalate stones (70%), uric acid (27%), phosphates (23%), struvite (4.9%). Carbonates (0.4%), cystine (1.5%), brushite (1.1%) were only rarely diagnosed. A spectral database of urinary stones of mixed type and in pure form was compiled, the spectra of which were obtained by ATR FT-IR spectroscopy method. It has been shown that the IR spectra recorded using the ATR FT-IR accessory can be successfully used to study the composition of urinary stones along with the IR transmission spectra in KBr pellets.

Acknowledgements: This work is a part of the Moldovan State Program (2020-2023) “Study and management of pollution sources to develop recommendations for implementing measures to mitigate the negative impact on environment and human health”, Project number: 20.80009.7007.20.

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PP1.13

Spectrophotometric method for quantitative determination of the drug "mabipan"

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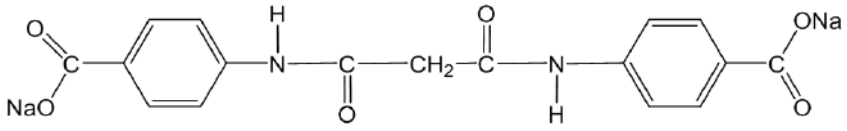
Mabipan (disodium salt of N, N'-malonyl-bis-p-aminobenzoic acid) was previously synthesized in Institute of Chemistry, pharmacologically studied and partially clinically tested. This drug was recommended for the treatment of a number of cardiovascular diseases. It was a sterile powder produced in vials: injection solutions of the drug were prepared ex tempore. The aim of our study was to develop an express method for the quantitative determination of the active substance, both in the substance and in the dosage form [1-3].



MABIPAN

When searching for methods for the quantitative determination of Mabipan, direct acid-base and potentiometric titration methods were tested. It was practically impossible to obtain consistent results with these methods, since the equivalence points of both carboxyl groups were stretched and did not coincide, which caused difficulties in determining the equivalence point. Precipitating the fine crystalline sediment of free N,N'-malonyl-bis-p-aminobenzoic acid that formed during potentiometric titration turned out to be a strong adsorbent for dissolved Mabipan. A pronounced absorption maximum in the region of 266.3 nm was detected during UV spectrophotometric study of an alkaline aqueous solution of Mabipan (pH = 9 – 9.5). The conformity of the absorption maximum to the Bouguer-Lambert-Beer law was revealed when preparing a series of solutions with concentrations in the range of 0.13 - 17.00 • 10^{-6} g/mL. The spectra were recorded in a cuvette with a layer thickness of 1 cm relative to the diluent solution with pH = 9.5. Statistical processing of the results of the analysis of solutions (n = 6) with concentrations in the range of 4.0 - 6.0 • 10^{-6} g/mL showed good convergence of the results, which indicated the suitability of the spectrophotometric method for the quantitative analysis of Mabipan. The relative error ε_x of the method was 1.35%.

The proposed spectrophotometric method was suitable for the quantitative determination of the drug Mabipan both in the substance and in the dosage form [1].

References

1. Şepeli D. Analiza şi standardizarea unor noi preparate medicamentoase cu aplicarea metodelor spectrale şi cromatografice. Autoreferat al tezei de doctor în ştiinţe chimice, Chişinău, 2008.
2. Darciuc, V., Ghicavîi, V., Parii, B. Hemodinamica sistematica în administrarea Mabipanului. Revista Farmaceutică a Moldovei. 1996. nr.1, p.24-28. ISSN 1812-5077.
3. Şepeli, F., Darciuc, V. Interacţiunea derivaţilor N,N-malonil-bis-acid P-aminobenzoic cu cationii de K, Mg şi Ca ca mecanism posibil al acţiunii lor cardiotrope. Revista Farmaceutică a Moldovei. 1995. nr.1, p.23-26. ISSN 1812-5077.

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PP1.14

Evaluation of antibacterial activity of 3*d* metal complexes with 1-(morpholin-4-yl)propane-1,2-dione 4-phenylthiosemicarbazone towards *Staphylococcus aureus*

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A 2022 WHO GLASS report noted *S. aureus* as the third-most prevalent bacterium worldwide. This bacterium has quickly adapted to newly developed antibiotics by evolving effective resistance mechanisms. The rise of bacterial strains resistant to antimicrobial agents is driven by several factors, including the overuse and misuse of antibiotics, their frequent application as growth promoters in livestock feed, and the growing ease of global travel, which facilitates the spread of resistant bacteria across regions and countries. Antimicrobial action of thiosemicarbazone's metal complexes is well-documented in the literature. So, the aim of this work is the study of antibacterial activity of some 3*d* metal complexes with 1-(morpholin-4-yl)propane-1,2-dione 4-phenylthiosemicarbazone (HL) towards microorganisms *Staphylococcus aureus*.

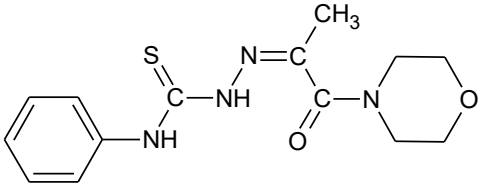

Fig. 1. The structure of HL.

The HL was obtained by the reaction between 1-(morpholin-4-yl)propane-1,2-dione and 4-phenylthiosemicarbazide in ethanol (Fig. 1) and was studied using ^{1}H, ^{13}C NMR and FTIR spectroscopies. The complexes $[Zn(L)_2]$, $[Ni(L)_2](NO_3)_2$, $[Co(L)_2]NO_3$, $[Co(L)_2]Cl$, $[Fe(L)_2]NO_3$ were obtained by reaction between HL and metal salts, and were studied using FTIR spectroscopy, elemental analysis and molar conductivity.

The antibacterial activity was studied towards *Staphylococcus aureus* (ATCC 25923) and the minimum inhibitory concentrations (MICs, μg mL^{-1}) and minimum bactericidal concentrations (MBCs, μg mL^{-1}) were determined using the method of serial dilutions in liquid broth. The activity of the complexes is influenced by the nature of their central metal atom and the activity decreases in the following order: $Co^{3+} > Ni^{2+} \approx Fe^{3+} > Zn^{2+}$. The most active one is complex $[Co(L)_2]Cl$ with MIC value 31.25 μg mL^{-1} and MBC value 31.25 μg mL^{-1}.

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PP1.15

Exploring the antifungal activity towards *Candida albicans* of copper(II) complexes with 2-benzoylpyridine 4-norbornylthiosemicarbazone

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Candida albicans is a highly adaptable microorganism, being able to develop resistance following prolonged exposure to antifungals. One of the main reasons *Candida* infections can be deadly is that they are hard to diagnose. The symptoms are not specific, lab tests take time, and this often leads to delays in starting the right antifungal treatment. Studies described in the literature prove that 2-benzoylpyridine thiosemicarbazones and their copper(II) coordination compounds exhibit antifungal properties. Based on all of the above, the aim of this work is the study of antifungal activity towards fungi *Candida albicans* for copper(II) complexes with 2-benzoylpyridine 4-norbornylthiosemicarbazone (HL).

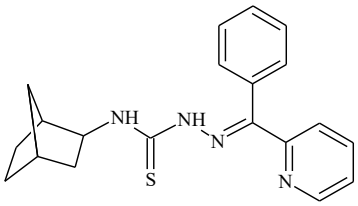

Fig. 1. The structure of HL.

The HL was synthesized in two steps (Fig. 1). First was the reaction between 4-norbornylthiosemicarbazide and 2-benzoylpyridine with HCl in ethanol, and the second was the neutralization of the obtained hydrochloride of HL with Na_2CO_3. The obtained HL was studied using ^1H, ^{13}C NMR, FTIR spectroscopies and X-Ray diffraction. The copper(II) complexes were synthesized by the reaction between HL and copper(II) salts in hot in 1:1 molar ratio. The complexes $[Cu(L)NO_3]$, $[Cu(L)Cl]$, $[Cu(L)CHCl_2COO]$ were studied using elemental analysis, FTIR spectroscopy and X-Ray diffraction.

The antifungal activity was studied towards fungi *Candida albicans* (ATCC 10231) the minimum inhibitory concentrations (MICs, μg mL^{-1}) and minimum fungicidal concentrations (MFCs, μg mL^{-1}) were determined using the method of serial dilutions in liquid broth. The activity of the obtained copper(II) complexes is influenced by the acid anion, and the antifungal activity decreases in the following order: $Cl^- \approx CHCl_2COO^- > NO_3^-$. The most active complexes $[Cu(L)Cl]$ and $[Cu(L)CHCl_2COO]$ manifest antifungal activity with MIC value 0.24 μg mL^{-1} and MFC value 1.95 μg mL^{-1}.

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PP1.16

Spectral studies on some dextran-iron oxide nanoparticle composites

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In this presentation, we report the spectral characterization of Fe_3O_4 nanoparticles coated with dextran. The structural and optical properties of the Dx:Fe_3O_4 synthesized composites were investigated by Fourier Transform infrared (FTIR) spectroscopy, X-ray diffraction (XRD) and UV-Vis absorption. Also, the photophysics of Dx:Fe_3O_4 composites is described using fluorescence and phosphorescence methods and the quantum yields and lifetimes of excited states were estimated. By using transient absorption spectroscopy, it was obtained ground state bleaching bands (**GBS**), absorption in excited state (**ESA**) and at longer wavelengths stimulated emission (**SE**). Dextran-iron oxide composites exhibit strong fluorescence in contrast to pure Fe_3O_4 NPs. Phosphorescence spectra confirm the formation of new emission bands within the Dx:Fe_3O_4 solution evidenced by the maxima shift for both, dextran and Dx:Fe_3O_4 composite. These features make as the prepared Dx:Fe_3O_4 composites to be applicable for drug delivery systems, bioimaging, organic solar cells and highly fluorescent hybrid materials. In this study, by analyzing the emission spectra, decay lifetimes, and energy states, we aim to provide a comprehensive understanding of the transitions and processes governing the optical response of Dx:Fe_3O_4 systems, and to contribute to the broadening of photophysics field by detailing how surface modifications, by dextran coating, influence the energy levels and emission properties of Fe_3O_4 NPs, ultimately enhancing their potential for applications in different fields.

Keywords: Dx:Fe_3O_4 composite, photophysics, fluorescence.

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PP1.17

HCl-induced opening of steroid epoxides: mechanism and products

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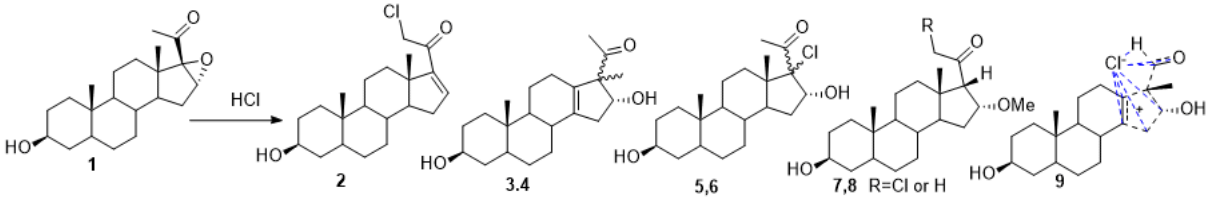
Steroid-based epoxides are valuable intermediates in the synthesis of pharmacologically relevant molecules, including imidazolium salts with anticancer potential [1]. In this study, we revisited a literature-reported method for the hydrogen chloride-mediated epoxide ring-opening of steroid (**1**) (see Scheme), which was originally designed to yield a single chlorinated compound (**2**) [2]. However, the original report also mentioned a minor "dimeric" byproduct of unknown structure. Importantly, the yield of the desired product was found to vary significantly with even slight changes in reaction parameters. To improve reproducibility, we investigated the underlying mechanism by systematically varying reaction conditions. Column chromatography consistently revealed eight reaction products, though their proportions changed with conditions. Among them were the expected chlorinated compound (**2**) and a major byproduct previously misidentified as a dimer. Detailed NMR analysis (1D and 2D techniques) showed this material to be a mixture of diastereomers (**3**, **4**) resulting from protonation-induced epoxide opening followed by skeletal rearrangement, with retention of configuration at the oxygen-bearing carbon and inversion at C-17—contradicting earlier mechanistic proposals. A minor chlorinated diastereomer (**5**) was isolated and fully characterized, while a second epimer (**6**) was identified in an enriched fraction. Both differed only in the stereochemistry at C-17. Additionally, two methanol adducts (**7**, **8**) were isolated, formed by anti-Markovnikov, *trans*-type addition to the *α,β*-unsaturated ketone intermediate. NOESY spectra confirmed spatial proximity between C-18 and 17*β*-H, supporting the proposed addition pattern.

Scheme



Based on these findings, we proposed a revised mechanism encompassing all observed products and side reactions. Remarkably, a speculative skeletal rearrangement involving C-21 methyl migration was supported by isolation and X-ray crystallography of a trace compound (**9**), confirming the formation of a 21-nor-steroid framework.

This study clarifies the complex reaction pathways involved in the HCl-induced opening of steroidal epoxides. It challenges earlier mechanistic assumptions and establishes a more accurate understanding of product formation. These insights enable more reliable synthetic access to structurally defined, bioactive steroid derivatives and could be pivotal for the rational development of steroid-based anticancer agents.

Acknowledgements: This research was carried out within the framework of the project "Chemical study of secondary metabolites from local natural sources and valorization of their applicative potential through the expansion of molecular diversity with multifunctional properties (MetNatVal)" (code: 010601).

References

1. Sucman, N. et al. Steroids, 210, 2024, 109475.
2. Girdhar, N., Ishar, M. Chem. Commun., 18, 2002, 2102–2103.

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PP1.18

Soluble nitrogen species in model of river or lake water samples as indicators of the state of the aquatic environment

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Ammonium, in particular, is of great concern due to its similarity to an amino acid, where a hydrogen atom is substituted with an organic radical containing a carboxylic group. Amino acids are the building blocks of proteins, the essential molecules supporting life processes. As a result, ammonium in aquatic environments can play a dual role: it can serve as a building block for the creation of living organisms and also provide energy support for the activities of aquatic organisms. Ammonium serves also as a universal catalyst for the emergence of a new state within the aquatic environment. Laboratory modeling involving by ammonium initiation is highly responsive to the presence of anthropogenic pollutants, such as surfactants, heavy metals, and the existence of antibacterial agents, among others. It can even detect variations in the different states of these pollutants within the aquatic (polluted) environment. Consequently, the discharged water into the natural water bodies often fails to meet these two crucial (trophic and environmental) waters quality indicators for a river. Starting from the pollution source (the city of Soroca, Republic of Moldova) along the water course, laboratory simulations easily highlight the degree of self-purification. For example, comparing the oxidation/formation/reduction process of nitrogen species (NH_4^+, NO_2^- and NO_3^-) in river water samples reveals a difference in samples subjected to the same modeling approach. This difference becomes even more pronounced when fine particles of calcium carbonate are added to the river water samples. The decomposition of complex compounds of anionic and cationic surfactants (SAS An · SAS Ct), and spatial reorientation, leads to a change in the self-cleaning process. This phenomenon is commonly observed in biological treatment technologies. In wastewater treatment plants (WWTPs), the phenomenon of inhibiting ammonium oxidation occurs, especially when oxidation did not occur at the initial stage of treatment, where both aerobic and anaerobic processes take place, involving the oxidation of ammonium ions, as well as the reduction of nitrates and nitrites returning from the final stage of the treatment process. Typically, in wastewater treatment plants (e.g., WWTP Chisinau), the emergence phenomenon is combined in the final stage with an inhibition of the oxidation and assimilation of both organic carbon and ammonia nitrogen. Therefore, the discharged water into the natural water bodies often fails to meet these two crucial water quality indicators for a river. Laboratory simulations conducted with river water samples exhibit sensitivity to the presence of various substrates, including different fractions of granite and spongy clay. These simulations reveal an acceleration in the oxidation of both ammonium and nitrite ions, underscoring the clear and beneficial effects of self-purification processes.

Acknowledgements: This work is a part of the Moldovan State Program (2024-2027) "Advanced research in computational and ecological chemistry, identification of technological procedures for treatment, formation of water quality and quantity", Project number: 010603.

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PP1.19

The synthesis of triazolium salts 2*h*-chromene-2-ol

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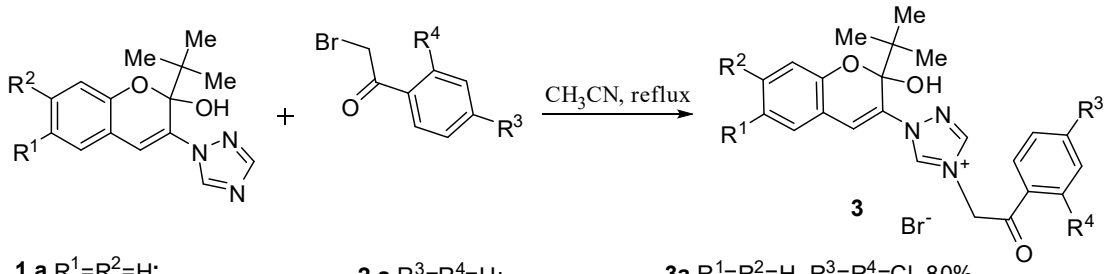
Chromene and triazole moieties are widely represented in a huge amount of biologically active molecules and semi-synthetic agents. Of interest are compounds containing fragments of several biologically active classes such as 1.2.4-triazoles [1] and chromenes [2]. To explore potential biologically active compounds in the series of 2H-chromen-2-ol derivatives, we have synthesized a series of heterocyclic compounds [3]. In this work, the possibility of obtaining salts for functionalization of biologically active chromene-triazole was investigated.

The present study was focused on the synthesis of designed biohybrids which were produced by the combination of chromene-triazole based and phenacyl bromide and its derevates. The chromene- triazole based moiety was employed as one of the substrate for grafting with phenacyl bromide for the generation of novel triazolium salts. The synthetic route, along with the reagents and conditions for the target compounds, is shown in Scheme.

A series of new salt derivatives consisting of bromides based on chromene-triazole and phenacyl in one chemical compound were designed and synthesized as potent bioactive compounds. The chemical structures of all the synthesized derivatives were determined by nuclear magnetic resonance (^{1}H NMR and ^{13}C NMR) and Fourier-transform infrared (FT-IR) spectral analysis.



1 a R^1=R^2=H;
1b R^1=Cl, R^2=H;
1**c** R^1=Br, R^2=H;
1**d** R^1=H, R^2=Ph;

2 a R^3=R^4=H;
2**b** R^3=Me, R^4=H;
2**c** R^3 =R^4=Cl

3a R^1=R^2=H, R^3=R^4=Cl, 80%
3b R^1=R^2=R^3=R^4=H, 60%
3c R^1=R^2=R^4=H, R^3=Me, 70%
3d R^1=R^4=H, R^2=Ph, R^3=Me, 60%;
3e R^1=H, R^2=Ph, R^3=R^4=Cl, 70%;
3f R^1=H, R^2=Ph, R^3=R^4=Cl, 70%
3g R^1=Cl, R^2=R^4=H, R^3=Me. 70%;
3h R^1=Cl, R^2=R^3=R^4=H, 88%;
3i R^1=Br, R^2=R^4=H, R^3=Me. 80%;

The antifungal activity of chromene-triazole salts was evaluated against different species: *Candida albicans, Saccharomyces cerevisiae. Aspergillus fumigatus*, *A. versicolor, A. ochramensis*, *Trichoderma viride* respectively. All the tested compounds exhibited good antifungal activity which was higher compared to the parent components and reference drugs (ketoconazole and bifonazole). Compound **3d** was patented and recommended for use in agriculture as an antifungal agent.

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References

1. Strzelecka, M., Swiatek, P. Pharmaceuticals, 2021, 14(3), 224. https://doi.org/10.3390/ph14030224
2. Cai Guangrong. et al. Chem. Res. Chinese Universities, 2019, 35(2), 221-228. https://doi.org/10.1007/s40242-019-8303-6
3. Zveaghintseva, M. et al. Molecules, 2021, 26, 4304. https://doi.org/10.3390/molecules26144304

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PP1.20

Antioxidant co-action of wine polyphenols and organic acids

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For decades, wine has been extensively studied for its antioxidant properties and associated health benefits [1]. Its high content of polyphenols – such as resveratrol and flavonoids – along with organic acids possessing antioxidant capacity, contributes to the neutralization of free radicals and supports the concept of the French Paradox [2]. Recent studies have shown that, within mixtures of antioxidants, various types of interactions can occur – synergistic, additive, or antagonistic – depending on factors such as concentration, solvent, pH, and mechanisms of action [3].

In this study, seven antioxidant compounds commonly found in wine – ascorbic acid (AA), dihydroxyfumaric acid (DHF), gallic acid (GA), and four natural polyphenols: catechin (Cat), quercetin (Que), rutin (Rut), and resveratrol (Res) – were used to investigate the nature of antioxidant interactions in wine. Twenty-one binary mixtures, each combining two antioxidants in a 1:1 ratio, were analysed using the DPPH assay [4].

Preliminary results indicate that mixtures containing AA and DHF exhibit predominantly synergistic effects, with the highest values observed for DHF–GA (1.17), DHF–Rut (1.11), DHF–Que (1.10), and AA–GA (1.10). Moderate synergism was also noted for AA–Rut (1.09), AA–Que (1.08), and Que–Rut (1.07). The most significant synergistic effect was found for the Que–GA combination (1.20), most GA-based mixtures showing either synergistic or additive interactions. In contrast, all combinations involving Res exhibited antagonistic effects, with values ranging from 0.83 to 0.92.

These findings are consistent with our previously published data on interactions between grape-derived polyphenols and organic acids [3], as well as on AA–DHF interactions [5]. Further research is needed to investigate these interactions in a simulated wine matrix, in order to better assess their impact on the antioxidant capacity and health-promoting potential of wine.

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References

1. El Rayess, Y., Nehme, N., Azzi-Achkouty, S., Julien, S. G. Antioxidants, 2024, 13(11), 1312.
2. Mitrović, D., Sredović Ignjatović, I., Kozarski, M., Popović-Đorđević, J. Food Safety and Health, 2024, 2(2), 196-212.
3. Vicol, C., Duca, G. Acta Chimica Slovenica, (2023), 70(4), 588–600.
4. Brand-Williams, W., Cuvelier, M. E., Berset, C. L. W. T. LWT-Food science and Technology, 1995, 28(1), 25-30.
5. Vicol, C., Fifere, A., Duca, G. Chemistry Journal of Moldova, 2024, 19(1), 29-36.

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PP1.21

New collagen-based membranes for glioblastoma treatment

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Recent studies demonstrate that a promising new treatment for glioblastoma, which could be rapidly implemented in the clinic, is represented by implants. Nanoengineering has shown enormous potential in the treatment of glioblastoma, and the collagen-based membranes proposed in this study represent an innovative therapeutic opportunity for the treatment of drug-resistant brain cancers.

Collagen-based membranes, which use medical collagen derived from bovine dermal waste and minocycline and irinotecan as useful drugs, were developed to specifically address high-grade glioma, the chosen substances being proven therapeutic agents for this type of central nervous system malignancy and collagen being a readily absorbable and degradable biopolymer. The results of this study showed that the type and concentration of the drug significantly influence the water absorption, enzymatic degradation, antimicrobial activity and drug release characteristics of the created membranes. The biphasic kinetic profiles are favorable for the prophylaxis and local treatment of glioblastoma, and drug release results suggest that the membrane containing 30-50% irinotecan continues to release the drug even after two days, while the membrane with 40% minocycline provides substantial drug concentrations in the first five hours and lower concentrations up to 24 hours.

The obtained results lead to the conclusion that these membranes could substantially improve the efficacy of localized treatment by optimizing initial release with extended drug availability, particularly in the context of antibiotic administration and the presence of chemotherapeutics. Therefore, the development of these membranes marks a significant step forward towards the formulation of a comprehensive treatment modality for the particular challenge of glioblastoma.

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PP1.22

Dihedral angles and conic projection under wave motion

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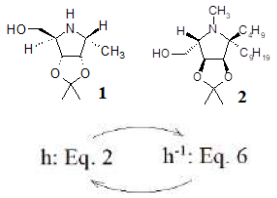
Dihedral angles [1,2] are calculated from differences between two atoms of carbon $\Delta\delta_{CnCn+1}$[ppm] with conic projection (eq. 1-3) [3] under Lie algebra and Hop fibration theories having 3-Sphere as model [4]. Since the wave character of NMR data ensure continue "deformation" into to other, r of cone is under homotopic behavior, *i.e.* eq. 2 with eq. 6.

Eq. 1: $\theta = \sec^{-1}h$, Eq. 2: $r = (h^2 - 1)^{1/2}/h$, Eq. 3: $z = \cos\theta = 1/h$

A method in 3 steps: 1. Calculation h of cone: from equation 4 result one angle of set A^{I}, and with equation 5 result h from first angle of set A^{I1}; 2. Calculation vicinal angles ϕ[deg] and or dihedral angle θ_{HnHn+1}[deg]: from eq. 6 or 3 and 7 results one angle of second sets A^{II} and B^{II}, sometimes directly vicinal or dihedral angles; 3. Calculation dihedral angles: angles of sets θ^{AII} and θ^{BII}[deg] are transformed in dihedral angles with characteristic equations for calculation dihedral angles θ_{HnHn+1}[deg] from vicinal angles[5]. The vicinal angle ϕ[deg] result in unit of seven set angles or from transformation between U to S [4]. Homotopic property under conic projection gives for a vicinal coupling constant $^3J_{H2H3}$ 7.3 [Hz] from eq. 2 a vicinal angle of 53.56[deg], and from eq. 6 a vicinal angle of 214.13[deg]. Conic projection under torus geometry was demonstrated with eq. 8.



Step 1: Eq. 4: $\cos^{-1}R_m = \theta^{AIn}$
$\theta^{AIn} \rightarrow \theta^{AI1}$, n = 1 - 6
Eq. 5: $\cos\theta^{AI1} = 1/h$

Step 2: Eq. 6: $r = [(1/h)^2-1]^{1/2}/(1/h)$
Eq. 7: $\sin^{-1}r = \theta^{AIIn}$
$\theta^{AIIn} \rightarrow$ units

where: θ^{AI1} – first angle of set A calculated from differences between two atoms of carbon $\Delta\delta_{CnCn+1}$[gaussx10]; θ^{AIIn} – one angle of set θ^{AII} in close relationship with set θ^{BII}, or directly dihedral θ_{HnHn+1}[deg] or vicinal angles ϕ[deg].

Eq. 8: $\cos^{-1}R_m = \theta^{ANn} = \sin^{-1}r$

Table 1: Vicinal angle ϕ[deg] and 3-Sphere dihedral angles θ_{HnHn+1}[deg] calculated with conic projection (Eq. 6) from differences in chemical shift between two atoms of carbon $\Delta\delta_{CnCn+1}$[deg] for imiocyclitols **1**, **2**.

	$^3J_{HH}$[a] [Hz]	Φ [deg]	δ_{CnCn+1} [gaussx10]	θ^{AIn} [deg]	θ^{AI1} [deg]	1/h [π]	r [π]	θ^{AII} [deg]	Φ [deg]	$^3J_{HH}$[calc] [Hz]	θ_{HnHn+1} [deg]
1	4.1	67.24, 16.81	0.7559	39.11	20.88	0.934	0.381	22.43	67.56	4.1	22.43, -24.38, -42.74
	5.4	116.64, 29.16	0.0224	88.71	28.71	0.547	0.547	33.41	116.78	5.40	-26.78, -41.75, 30.31
	0		0.5154	58.97	1.024	0.999	1.1432	88.85	1.143	0.534	-88.97, -91.143
2	7.3	213.16	0.112	83.56	23.56	0.916	0.436	25.86	214.13 212.29[b]	7.31 7.28	-55.87, -42.67, 29.29 -57.93, -38.78, 27.96
		53.29	0.112	83.56	23.56	1.090[h]	0.3998	23.56	53.566	7.31	36.43, -38.81, -47.57
	4.5	81, 20.25	0.3417	70.01	10.01	0.984	0.176	10.17	20.34 80.68	4.51 4.49	69.65, -21.76, -19.17 9.31, -9.43, -44.61

a. $CDCl_3$, δ[ppm]: ^{1}H 400[MHz], ^{13}C 75[MHz], b. r = 0.436[radieni] – r^{-1} = 2.29[deg].

Alternatives methods used to date calculate h^{AI} to h^{AN} until the calculated value is closed to recorded one [6,7]. A method with applications on conformational and configurational analysis [8].

References: **[1]** C.-I. Mitan, E. Bartha, F. Petru, C. Draghici, M.-T. Caproiu, R. M. Moriarty, Rev. Roum. Chim. 2023, 68(3-4), 185; DOI: 1-.33224/rrch.2023.68.3-4.08; **[2]** C.-I. Mitan, E. Bartha, P. Filip, C. Draghici, M.-T. Caproiu, R. M. Moriarty, Science J. Chem. 2024, 12(3), 42; doi.org/10.11648/j.sjc.20241203.11; **[3]** E. W. Weisstein, httpd://mathword.wolfram.com/ConicProjection.html; **[4]** C. I. Mitan, E. Bartha, P. Filip, R. Moriarty, chapter book: Dihedral and tetrahedral angles of five and six membered ring calculated from NMR data with 3-Sphere approach, IntachOpen 2025 ISBN 978-1-83635-220-4; doi.hhtp://dx.doi.org/10.5772/intechopen.1009208; **[5]** C.-I. Mitan, E. Bartha, P. Filip, C. Draghici, M.-T. Caproiu, R. M. Moriarty, ACS Spring, San Diego march 23 – 27, CARB 623, ID 4175487; doi.org/10.1021/scimeetings.5c11051; **[6]** C.-I. Mitan, R. Moriarty, P. Filip, E. Bartha, M. T. Caproiu, C. Draghici, 256th ACS Boston, MA, August 19-23, 2018, CARB 84, ID: 2972261, 51 pag; **[7]** C.-I. Mitan, E. Bartha, F. Petru, C. Draghici, M.-T.Caproiu, R. M. Moriarty, Science J. Chem. 2023, 11(6), 212; doi:10.11648/j.sjc.20231106.12; **[8]** C.-I. Mitan, P. Filip, E. Bartha, C. Draghici, M.-T. Caproiu, R. M. Moriarty, ACS San Diego march 23-27, Sci-Mix CARB – ANYL 632, ID 4175485; doi.org/10.1021/scimeetings.5c11052.

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PP1.23

Reduced forms of oxygen and their role in the redox-catalytic reactions *in vivo*

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Activation of the dioxygen molecule due to its complex formation with the transition metal ions (mainly, Fe, Cu, Mn, Co, Zn, etc.) is one of the possible pathways of organic substrates oxidation - an energetically advantageous catalytic process. This complex formation leads to the redistribution of electronic density of interacting components and formation of oxy-radicals ($^1O_2$, $HO_2^\bullet$, $O_2^{\bullet-}$, $OH^\bullet$) as well as a series of intermediate particles [1]. The products of dioxygen reduction are existing within the cells and intercellular liquids in the strictly defined and limited concentrations, which are controlled by the strong enzymatic and other regulating systems. Various internal and external effects violate such control, which can induce the oxidative stress leading to cells death [2]. The other ways of free radicals generation in the cells and tissues can be radiation (UV, vis, thermal, ionizing), or enzymatic processes.

One of the dioxygen molecule activation products, superoxide-radical $O_2^{\bullet-}$, although not a strong oxidant, is capable, due to the Haber-Weiss reaction, to generate the strongest oxidant – hydroxyl-radical $OH^\bullet$. An excessive extracellular generation of superoxide-raidcals *in vivo* can bring out the specific „response" of mammal organisms in the form of inflammatory process, thus initiating the launch of neutrophil activation [2].

The oxygen-based free radicals, occurring in significant amounts in living organisms, provoke the state of toxicity. The $O_2^{\bullet-}$ radical is one-electron oxidizer and iron complexes can modify their oxidation states, forming the pairs LFe(III)/LFe(II), or LFe(IV)/LFe(III), as in the case of active centers of peroxidase. Thus, if the L ligands are active σ-donors, the redox potential of the LFe(IV)/LFe(III) pair could be decreased, which facilitates the stabilization of more oxidized state, i.e. Fe(IV). It suggests that the unique toxicity of superoxide-radical is stipulated by its capacity to induce the site-specific generation of highly-oxidized and metal particles with high potential of self-destruction [3].

The processes causing the toxicity of the reduced oxygen forms are still under discussion and require further studies. This is important because the reactive free radicals can *in vivo* damage the DNA, destroy the nucleotide co-enzymes, affect the SH-dependent enzymes and membranes, trigger lipid peroxidation (LPO) and other catalytic and non-catalytic reactions accompanied with the damage of cells, provoking the occurrense of numerous diseases (oxidative stress-related diseases, inflammatory processes, atherosclerosis, myocardial ischemia, aging-related diseases).

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References

1. Duca Gh. (2012). Homogeneous Catalysis with Metal Complexes: Fundamentals and Applications. Berlin, Heidelberg: Springer, 478 p. https://www.springer.com/gp/book/9783642246289.
2. Yu Y., Cui Y., Niedernhofer L., and Wang Y. (2016). Occurrence, biological consequences, and human health relevance of oxidative stress-induced DNA damage. Chemical Research in Toxicology. 29(12), 2008–2039, https://doi.org/10.1021/acs.chemrestox.6b00265.
3. Andrés, C. M. C., Pérez de la Lastra, J. M., Andrés Juan, C., Plou, F. J., & Pérez-Lebeña, E. (2023). Superoxide Anion Chemistry—Its Role at the Core of the Innate Immunity. International Journal of Molecular Sciences, 24(3), 1841. https://doi.org/10.3390/ijms24031841.

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PP1.24

oxidative polymerization of ortho-phenylenediamine and 1,4-benzenediol: a route to nano-sized oligomers

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Oxidative polymerization of aromatic amines and phenols has attracted much attention due to its ability to form homo- and co-oligomers with a conjugated system with an interesting set of properties (physicochemical and electronic properties). In this regard, the oxidative polymerization of ortho-phenylenediamine and 1,4-diaminobenzene is of particular importance.

A novel nano-sized co-oligomer based on o-phenylenediamine (OPD) and 1,4-benzenediol (1,4-BD) has been synthesized through oxidative polymerization at room temperature in an acidic (HCl) medium, using potassium persulfate ($K_2S_2O_8$) as the oxidizing agent.

The structural, thermal, and morphological properties of the synthesized compound were examined using FTIR, UV–Vis, TGA, SEM, and ESR spectroscopies. The copolymerization mechanism of OPD with 1,4-BD monomers has been proposed.

The FTIR spectrum exhibited characteristic absorption peaks. The strong absorption bands at 3301 (broad) and 3133 cm^{-1} are due to O-H and N-H stretching vibrations, respectively, indicating the presence of hydroxyl and secondary amine groups in the compound. Another strong signal at 1612 and 1523 cm^{-1} represents the benzenoid (C=C) stretching vibrations of aromatic rings, confirming a conjugated system. The region from 886 to 724 cm^{-1} shows prominent C–H out-of-plane bending.

The UV–Vis data of the sample display strong absorption bands at 295 and 420 nm, linked to $\pi \rightarrow \pi^*$ and $n \rightarrow \pi^*$ transitions, respectively.

Electron spin resonance (ESR) spectroscopy was used to identify the unpaired electrons in the compound. The ESR spectrum consists mainly of a resonance line with g-factor

$g = 4.219 \pm 0.003$ and a resonance line width at high-height $\Delta B_{pp} = (8.4 \pm 1.3)$ mT. These date proof that there is no single electron within compound.

Additionally, the composite morphology, visualized by scanning electron microscopy (SEM), shows that the product consists of uniform nanoparticles. The thermogravimetric analysis (TGA) revealed that the synthesized compound has high heat resistance.

The proposed copolymerization mechanism of ortho-phenylenediamine (OPD) with 1,4-benzenediol (1,4-BD) indicates the formation of conjugated, electron-rich systems. The synthesized compounds are brown solid powder, soluble in polar organic solvents.

Overall, the analysis data confirms the successful synthesis of a conjugated nano-sized co-oligomer featuring both amino and hydroxy aromatic groups. These co-oligomers have potential applications in optoelectronic and sensing devices because of their unique features.

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PP1.25

DFT study of photoswitching systems based on fluorescent azulenyl-substituted dithienylcyclopentenes

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Organic molecular photoswitches combining dithienylcyclopentene with the azulene moiety represent an innovative class of photoactive compounds with applications in molecular electronics, optical sensors and smart materials [1-2]. The combination of these two components allows molecular switching between isomeric forms (open/closed) upon exposure to UV or visible light.

DFT study is used to determine the cyclization conditions, structural and electronic factors responsible for the specific properties of these compounds and the role of substituents.

Preliminary computational studies have demonstrated that in the case of some derivatives, such as bromo-azulene, the cyclization reaction is energetically favorable, the difference being 5.25 kJ/mol (Figure 1).

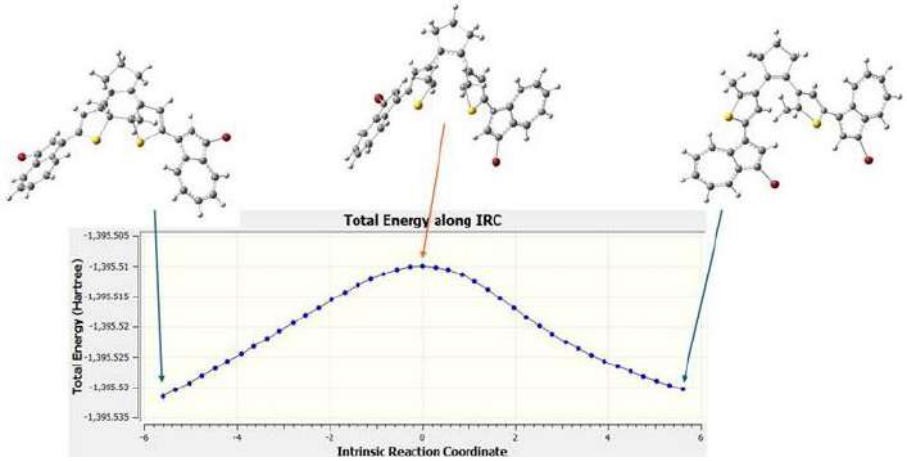

Fig. 1. Energy pathway for the cyclization reaction of 1,2-bis(5-(3-bromoazulen-1-yl)-2-methylthiophen-3-yl)cyclopent-1-ene

Funding
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References

1. Dragu E. A., Ion A.E., Shova S., Bala D., Mihailciuc C., Voicescu M., Ionescu S., Nica S., RSC Adv., 2015, 5, 63282;
2. Hou I.C.-Y., Berger F., Narita A., Müllen K., Hecht S., Angew. Chem. Int. Ed., 2020, 59, 18532.

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PP1.26

Copper(II) complexes of *syn*-2-pyridinealdoxime ligand for prospective biological applications

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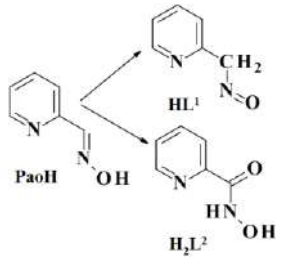
The focus of research in this field has recently been directed towards copper(II) coordination complexes with *syn*-2-pyridinaldoxime type ligands. These complexes possess structural diversity and versatility and, secondly, perhaps more importantly, they exhibit biological activity and potential for biological applications [1]. These compounds frequently exhibit diverse geometries of coordination polyhedra, redox properties and the ability to interact with biomolecules. Recent studies have indicated that such complexes may possess antibacterial, antifungal [1,2] or anticancer properties [3]. This phenomenon is primarily attributable to the redox activity of copper ions, in conjunction with the presence of ligands that bear donor nitrogen and oxygen atoms. The present study focuses on the copper(II) complex with *syn*-2-pyridinoxime (PaoH), which also contains a bridging ligand 4,4′-bipyridine (bpy). The crystal structure of the compound was determined by single crystal X-ray diffraction. The ionic compound $\{[Cu_4(L^1)_2(L^2)_2(bpy)_2](NO_3)_2 \cdot 2dmf \cdot 4H_2O\}_n$ (**1**) is based on one-dimensional cationic polymer $[Cu_4(L^1)_2(L^2)_2(bpy)_2]^{2+}{}_n$. The PaoH ligand, which is involved in forming the coordination polyhedra of two independent metal atoms (Cu(1) and Cu(2)), was found to undergo a chemical transformation *in situ*. This led to the formation of two different ligand derivatives: HL^1 and H_2L^2 (Scheme 1). While the Cu(1) and Cu(2) atoms exhibit square-pyramidal geometry dictated by N_3O_2 donor atoms, it should be noted that this set encompasses oxygen and nitrogen atoms from different ligands, $(L^1)^-$ and $(L^2)^{2-}$, as well as bpy (Fig. 1). In this case, the $(L^1)^-$ ligand is tridentately coordinated to two metal atoms, and $(L^2)^{2-}$ is tetradentately coordinated to three metal atoms.



Scheme 1. Ligand transformations of PaoH in compound **1**

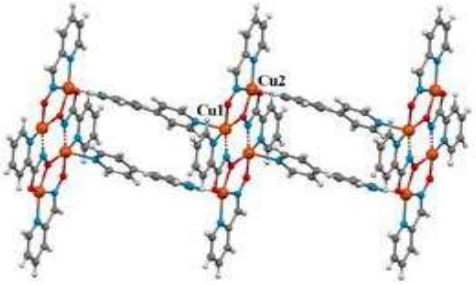


Figure 1. Fragment of 1D chain of $[Cu_4(L^1)_2(L^2)_2(bpy)_2]^{2+}{}_n$

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References

1. Coropceanu E.B., et. al. Synthesis and Structure of Mononuclear Zinc Complexes with Pyridine-2-Aldoxime. Russian Journal of Coordination Chemistry, 2017, vol. 43, pp. 278–285. Doi:10.1134/S1070328417050025
2. Hassan, E.A., Ebrahium, M.M., Ebrahium, A.M. Metal complexes of hydrazone-oxime derivative as promising in vitro antimicrobial agents against some fungal and bacterial strains. Applied Organometallic Chemistry, 2022, vol. 36. pp. 1-18. Doi:10.1002/aoc.6663
3. Alinaghi M., A Pd(II) complex derived from pyridine-2-carbaldehyde oxime ligand: Synthesis, characterization, DNA and BSA interaction studies and in vitro anticancer activity. Journal of Molecular Structure, 2020, vol. 1219, pp. 128479 Doi:10.1016/j.molstruc.2020.128479.

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PP1.27

Exploring limitations of 2D NMR quantitative experiments: variability of HSQC data depending on NMR probe and magnet power

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Quantitative NMR (qNMR) is a widely accepted method for ascertaining the concentration of one or more chemical species in solution by measuring the area of well resolved NMR peaks of the analyte and correlating the values against a known internal or external standard. For complex mixtures very congested 1D NMR spectra hinder the application of the1D qNMR experiments, and 2D experiments come to provide acceptable solutions. However, due to several experimental biases, qNMR through 2D experiments is very challenging and require a more rigorous approach for quantitation [1]. Normally, 2D NMR cross-peak volumes are strongly dependent on a set of factors, including T1 and T2 relaxation times and J-values, equipment parameters and recording conditions. We report in the current communication an exploratory study on the influence of the NMR equipment configuration on the variability of the quantitative HSQC data. The investigated mixtures represented extracts of 9 plants belonging to *Lamiaceae* family. The quantitative HSQC experiments have been performed on Bruker Avance III 400 (BBO), Bruker Avance Neo 400 (BBFO, BBI) and Bruker Avance Neo 600 (BBI) spectrometers, equipped with corresponding probes. Simultaneous quantitative determination of most abundant organic acids with phenolic and triterpenic structures has been performed according to a relative calibration protocol on the use of methyl 4-nitrobenzoate as internal standard. The convergence of quantitative data has been monitored on application of different number of scans, compatible with a routine laboratory analytical protocol. The quantitation was performed basing on a single calibration curve and all instruments' configurations showed convergent results. Processing of spectra was performed with Bruker Topspin software. It was observed that spectral processing parameters played a significant role in the measurement accuracy. Manual phase correction and automatic integration of diagnostic signals with relative threshold values provided best results. The obtained results demonstrate the feasibility of the method transfer between different NMR equipment within mandatory validation procedures.

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References

1. Giraudeau, P. (2017). Challenges and perspectives in quantitative NMR. Magnetic Resonance in Chemistry, 55(1), 61-69.

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PP1.28

Determination of rosmarinic acid in salvia species. Comparison of quantitative NMR and HPLC data

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Sage (*Salvia* sp.) is a widespread aromatic plant known for its multiple applications at global scale. The most known representatives are *Salvia Officinalis* (common sage) and *Salvia sclarea* (clary sage) exploited broadly for both therapeutical use and essential oil production. Rosmarinic acid is one of the main antioxidant constituents found in salvia species [1] and its reliable quantification represents a strong support for practical applications. In the continuation of our studies on the content of relevant secondary metabolites in European vegetal sources, we report in the current communication a comparative NMR – HPLC study of rosmarinic acid content in *Salvia Officinalis, Salvia Sclarea* and *Salvia Glutinosa* aerial parts collected in the central area of the Republic of Moldova and in the Neamț county of Romania.

Plant extracts have been obtained from aerial parts on ultrasound assisted extraction with 70 % aqueous ethanol. Quantitative NMR determination included HSQC experiments in accordance to the reported procedure [2]. HPLC determinations have been performed on an Agilent 1100 chromatographic system, consisting of a quaternary pump, autosampler and UV detector set at 210 nm. A Phenomenex Luna C18 column packed with 5 μm particles (150 × 4.6 mm LT× ID) ensured a satisfactory separation of rosmarinic acid under a gradient elution with aqueous TFA-methanol mixtures. A five-point calibration protocol has been applied, the method has been validated for linearity, repeatability, recovery and robustness.

The quantitative determinations showed very close results obtained by NMR and HPLC. The NMR results tended to show slightly lower values (85%) than HPLC, which can be attributed to chromatographic peaks overlapping with unresolved components. The content of rosmarinic acid reached the highest value in the crude extract of *Salvia Officinalis* and lowest in the similar extract of *Salvia Glutinosa*. These results confirm the validity of the NMR method for the quantitative estimation of lavender extracts within various biomedical and industrial applications and demonstrates the high potential for exploitation of antioxidants from sage related products.

Acknowledgments: This study was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS-UEFISCDI, contract no. 30ROMD/2024, project PN-IV-P8-8.3-ROMD-2023-0249 (DiMoMeD).

References

1. Anagnostou, M., Tomou, E. M., Krigas, N., & Skaltsa, H. (2025). Phenolic constituents of Greek native Salvia species: a comprehensive review. Phytochemistry Reviews, 1-81.
2. Girbu, V., Organ, A., Grinco, M., Cotelea, T., Ungur, N., Barba, A., & Kulcitki, V. (2023). Identification, quantitative determination and isolation of pomolic acid from lavender (*Lavandula angustifolia* Mill.) wastes. Sustainable Chemistry and Pharmacy, 33, 101140.

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PP1.29

Quantitative determination of rosmarinic acids in oregano extracts. A comparative study of NMR and HPLC data

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Oregano (*Origanum* spp.) is one of the most widespread plants of *Lamiaceae* family. The remarkable antioxidant activity of oregano derived products far exceeds other natural foods (12 times higher than orange, 30 times than potato, 42 times than apple) and is connected to the content of rosmarinic acid - a major secondary metabolite of polyphenolic structure [1]. In this line, the rosmarinic acid quantitative determination is a mandatory prerequisite in the perspective of a broader exploitation of oreganum species. In the continuation of our studies on the content of relevant secondary metabolites in European vegetal sources, we report in the current communication a comparative qNMR – HPLC study of rosmarinic acid content in two oregano varieties (*O. vulgare* and *O. vulgare ssp. hirtum*).

Plant extracts have been obtained from aerial parts on ultrasound assisted extraction with 70% aqueous ethanol. Quantitative NMR determination included HSQC experiments in accordance to the reported procedure [2]. HPLC analysis has been performed on an Agilent 1100 chromatographic system equipped with a UV detector set at 210 nm. A Phenomenex Luna C18 column packed with 5 μm particles (150 × 4.6 mm LT× ID) ensured a satisfactory separation of rosmarinic acid under a gradient elution with aqueous TFA-methanol mixtures.

The results of quantitative determinations showed very close values for both methods. The qNMR results tended to show slightly higher rosmarinic acid content (111 %) than HPLC for *O. vulgare ssp. hirtum*, and lower (87 %) for *O. vulgare* which can be attributed to chromatographic peaks overlapping with unresolved components. The content of rosmarinic acid proved to be higher in the crude extract of *O. vulgare* by both methods. These results confirm the validity of the NMR method for the quantitative estimation of oregano extracts within various biomedical applications and demonstrates the high potential for exploitation of antioxidants from oregano grown in the Republic of Moldova.

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References

1. Anagnostou, M., Tomou, E. M., Krigas, N., & Skaltsa, H. (2025). Phenolic constituents of Greek native Salvia species: a comprehensive review. Phytochemistry Reviews, 1-81.
2. Girbu, V., Organ, A., Grinco, M., Cotelea, T., Ungur, N., Barba, A., & Kulcitki, V. (2023). Identification, quantitative determination and isolation of pomolic acid from lavender (*Lavandula angustifolia* Mill.) wastes. Sustainable Chemistry and Pharmacy, 33, 101140.

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PP1.30

Selective anticancer activity of mixed-ligand copper(II) complexes with salicylaldehyde 4-allyl-*S*-methylisothiosemicarbazone

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The urgent global need for more effective and selective anticancer agents has driven extensive research into metal-based coordination compounds. In particular, mixed-ligand copper(II) complexes with heterocyclic amines have demonstrated promising cytotoxic and selective activity against various cancer cell lines. The synthesis of mixed-ligand copper(II) complexes with salicylaldehyde 4-allyl-*S*-methylisothiosemicarbazone (HL, Fig. 1) and various mono- and bidentate amines (pyridine, 3-picoline, 4-picoline, 3,4-lutidine, imidazole, 1,10-phenanthroline) has been carried out to investigate the influence of amine coordination on their anticancer activity. Structural analysis by FTIR spectroscopy, elemental analysis, and single-crystal X-ray diffraction confirmed that HL coordinates as a tridentate monoanionic NNO-donor ligand via the deprotonated phenolic oxygen, azomethine nitrogen, and thioamide nitrogen atoms. The sulfur atom does not participate in coordination.

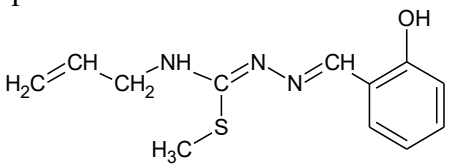

Fig. 1. The structure of HL.

The anticancer activity of the synthesized complexes was evaluated against HeLa (cervical carcinoma), BxPC-3 (pancreatic adenocarcinoma), and RD (rhabdomyosarcoma) cancer cell lines, as well as MDCK (normal dog kidney) cells to determine selectivity. The results demonstrated significant cytotoxic effects in the micromolar range (0.1–100 μM), with remarkable selectivity indices (SI) compared to Doxorubicin. Notably, the $Cu(Im)(L)NO_3 \cdot H_2O$ complex exhibited six-fold higher activity against HeLa cells than doxorubicin, with an SI of 4.48. Furthermore, $Cu(3\text{-}Pic)(L)NO_3 \cdot H_2O$ and $Cu(Im)(L)NO_3 \cdot H_2O$ demonstrated enhanced selectivity towards RD cells, exhibiting IC_{50} values of 2.8 μM and 1.33 μM, respectively. Notably, their selectivity indices, calculated as the ratio of cytotoxicity in MDCK cells to RD cells, were 4.57 for $Cu(3\text{-}Pic)(L)NO_3 \cdot H_2O$ and 7.07 for $Cu(Im)(L)NO_3 \cdot H_2O$, indicating significant preferential cytotoxicity against the cancerous RD cell line.

The cytotoxicity profile indicates that substitution of methyl groups in the pyridine ring reduces activity, while the introduction of bidentate ligands such as 1,10-phenanthroline enhances cytotoxic properties. The selective anticancer activity of these copper(II) complexes highlights their potential as promising agents with low toxicity toward normal cells.

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PP1.31

Synthesis and biological activity of novel coumarin and flavonoid derivatives: a structure-based approach

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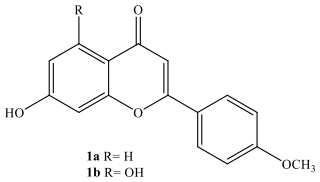
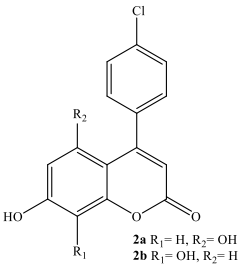
Flavonoids and coumarins are two prominent classes of plant-derived phenolic compounds with a wide range of biological activities, stemming from their distinct but related chemical structures. Their bioactivity is largely determined by their ability to interact with biological molecules and to modulate cellular processes. These class of compounds are well-known antioxidants, using their hydroxyl groups to scavenge free radicals and mitigate oxidative stress. However, at higher concentrations, they can exhibit a dual, prooxidant role by chelating metal ions, which can catalyze the formation of new, damaging free radicals [1].

The structure-activity relationship of these novel coumarin and flavonoid derivatives was investigated through their synthesis and biophysical characterization. The flavonoid derivatives were synthesized using DMAP as a catalyst, which enabled a regioselective pathway that preferentially formed the target product [2]. The coumarin derivatives were obtained via the Pechmann condensation in the presence of 78% H_2SO_4 [3].

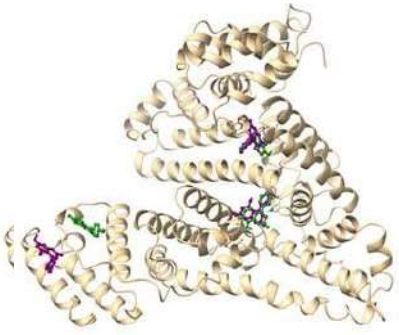
The interaction of compounds with DNA was confirmed by a concentration-dependent decrease in fluorescence, indicating that they successfully displaced the SYBR GREEN dye. Furthermore, the binding site of the coumarin derivative 2a within human hemoglobin was identified. The compound's calculated affinity is 9 μM, and its hydroxyl group forms a specific contact with a heme propionate [4,5].



1a R= H
1b R= OH



2a R_1= H, R_2= OH
2b R_1= OH, R_2= H



References

1. S.V. Jovanovic, S. Steenken, M. Tosic, B. Marjanovic, M.G. Simic, J. Am. Chem. Soc., 1994, 116, 4846-4851, doi.org/10.1021/ja00090a032
2. R. Kshatriya, V. P. Jejurkar, S. Saha, Tetrahedron, 2018, 74(8), 811-833, doi.org/10.1016/j.tet.2017.12.052.
3. D. S. Jang, E. J. Park, Y.-H. Kang, M. E. Hawthorne, J. S. Vigo, J. G. Graham, F. Cabieses, H. H. S. Fong, R. G. Mehta, J. M. Pezzuto, A. D. Kinghorn, J. Nat. Prod. 2003, 66, 9, 1166–1170, doi.org/10.1021/np0302100
4. N. Andrian, C. Zagrean-Tuza, M. Lehene, B. Brem, E. Gal, B. Stoean, L. Gaina, E. Hey-Hawkins, R. Silaghi-Dumitrescu, accepted for publication, doi:10.17632/kvbhc8yr2g.1.
5. M. Cosprundan, N. Andrian, C. Zagrean-Tuza, M. Lehene, B. Brem, E. Gal, A. Lupan, R. Silaghi-Dumitrescu, accepted for publication, doi:10.17632/98t5ff6d8j.1

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PP1.32

Zn(II) and Cu(II) complexes with a TMS-substituted indolo[2,3-*c*]quinoline Schiff Base – properties and cytotoxicity

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The isosteric exchange of carbon with silicon ("carbon-silicon switch") in known drug structures or the attachment of a trimethylsilyl (TMS) group to biologically active scaffolds may be a promising strategy for the development of novel drug candidates.

In this study, we report the multistep synthesis of the 9-trimethylsilylindolo[2,3-c]quinoline-derived Schiff base (**HLTMS**) and its Cu(II) and Zn(II) complexes, **Cu(HLTMS)Cl_2** (**1**) and **Zn(HLTMS)Cl_2** (**2**), their thorough characterization using elemental analysis, ESI mass spectrometry, single-crystal X-ray diffraction (SC-XRD) for **1**, spectroscopic techniques (IR, UV-Vis, ^{1}H and ^{13}C NMR for **HLTMS** and **2**), and electron diffraction (ED) for **2**.

The attachment of the TMS group increased the lipophilicity of **HLTMS** while complex formation with Cu(II) substantially improved the antiproliferative activity. Both HLTMS and the Zn(II) complex **2** produced reactive oxygen species under cell-free conditions, consistent with their redox activity as determined by cyclic voltammetry. The photochemical activity of the proligand and its complexes **1** and **2** has also been reported. The compounds exhibited significant toxicity on various human cancer cells and disrupted the mitochondrial membrane potential, suggesting the contribution of mitochondrial dysfunction, triggered by **HLTMS** and its metal complexes, to their toxic effects. Silylation in combination with the introduction of functional groups that increase the solubility of both the proligand and its metal complexes might allow full exploration of the potential of these kinds of compounds as photosensitizers in photodynamic therapy. These results underscore the potential of TMS-substituted Schiff bases as promising candidates for anticancer drug development.

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References

1. Wittmann, C., Besleaga, I., Mahmoudi, S., Palamarciuc, O., Balan-Porcarasu, M., Dascalu, M., Shova, S., Cazacu, M., Kiricsi, M., Igaz, N., Dömötör, O., Enyedy, E. A., Dvoranová, D., Rapta, P., Arion. V. B. Dalton Trans., 2025, 54, 7882–7898.

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PP1.33

Conjugated platinum(IV) complexes, potential prodrugs in cancer therapy

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New multifunctional platinum (IV) coordination compounds were designed to overcome the current limitations of platinum-based anticancer drugs, including side effects and resistance via drug efflux transporters, as well as an inability to effectively target cellular mechanisms. These new complexes were developed from platinum (II) cisplatin-type scaffolds by using additional therapeutic/diagnostic agents as ligands. This produced multifunctional therapeutic candidates with the potential to act as prodrugs, enhancing selectivity while limiting toxicity and enabling theranostics. The new complexes were characterized using state-of-the-art investigative techniques, including nuclear magnetic resonance (NMR) spectroscopy, mass spectrometry, and electrochemistry. Their antiproliferative activity was also investigated on different types of cancer cells such as MDA-231 și BT-549.

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PP1.34

Experimental and theoretical approaches to the biological activity of some Schiff bases and derived cobalt complexes

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Co(II) complexes with Schiff bases are considered biomimetic compounds for proteins that transport and store oxygen. Studies on the mechanism by which the oxygenation of cobalt complexes takes place have shown that the electron density on the central cobalt atom plays an important role in this process [1]. The influence of changing the in-plane ligand substituents on the cobalt-oxygen geometry was also studied [2]. Although there have been many studies on oxygen adducts of such complexes, few 1:1 complex: oxygen adduct structures have proven to be stable at room temperature. Therefore, it is of interest to isolate such a complex in a stable state and characterize it [2]. From another perspective, cobalt complexes seem to become an alternative in chemotherapy to those of platinum, whose use has become more restrictive due to toxicity and drug-resistant properties. Cobalt has been found to be less dangerous to the human body than platinum. A Co(III) complex with a Schiff base called Doxovir is even in an advanced antiviral clinical testing phase [3].

In this paper, we studied the biological activity of a cobalt complex of a salen-type Schiff base [4], which, compared to other complexes of this class reported in the literature, is distinguished by the presence in the structure of a highly flexible and hydrophobic siloxane spacer. The binding mode was predicted by molecular docking, some of these modes being illustrated in Figure 1.

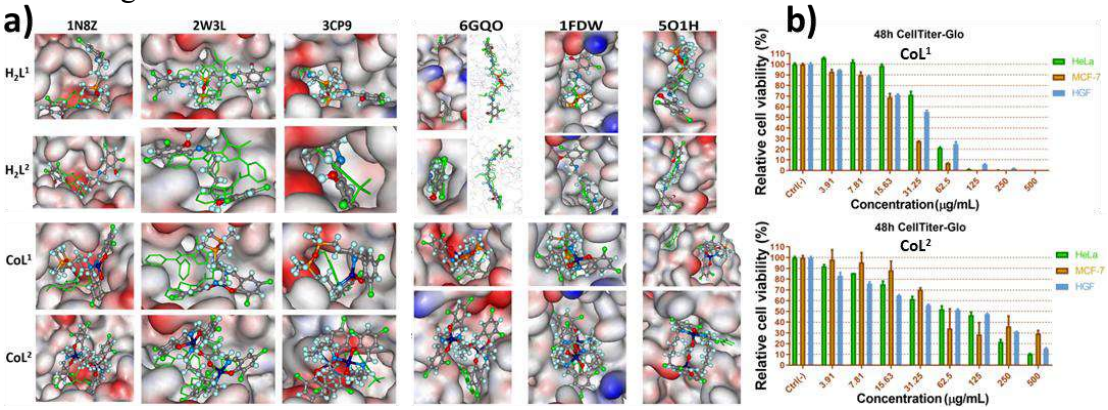

Figure 1. a) The docked pose of studied compounds (ball-and-stick) in different protein binding sites; the co-crystalized ligand is shown in line format (green); b) The effect of CoL1 and CoL2 on studied cell lines

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References

1. M. J. Carter, D. P. Rillema, F. Basolo, Journal of the American Chemical Society, 1974, 96, 392–400.
2. B. T. Huie, R. M. Leyden, W. P. Schaefer, Inorganic Chemistry, 1979, 18, 125–129.
3. K. Kanisha, G. Diya, K. Bikash, C. Chandra, Polyhedron, 2022, 222, 115890.
4. M. Damoc et al., Royal Society Open Science, 2025, 12, 250279.

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PP1.35

Synthesis, crystal structure and characterization of cobalt(II) coordination polymer derived from a 1,2,3-triazole-based tricarboxylate ligand

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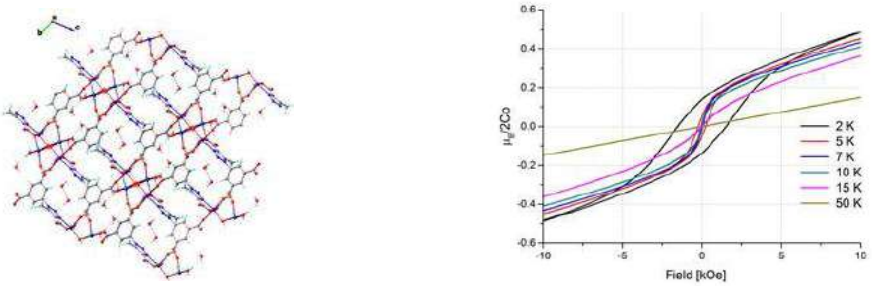
A novel three-dimensional homometallic coordination polymer formulated as $\{[Co_4L_2(H_2O)_2]\cdot 3H_2O\}_n$ (1) [H_3L = =5-(4-carboxy-5-methyl-1H-1,2,3-triazol-1-yl)isophthalic acid] was successfully synthesized by the reaction of H_3L with cobalt nitrate tetrahydrate, in a mixture of dimethylacetamide and water. In a few days pale-beige crystals were isolated and characterized by physical methods.

In the FTIR spectrum of **1** the characteristic bands for the carboxylate group appear at 1616 and 1456 cm^{-1} (absorbtions for the asymmetric $\nu_{as}(COO^-)$ and symmetric stretching $\nu_s(COO^-)$ vibrations of C=O bond). The absorbtion band appearing at 1377 cm^{-1} confirms the presence of the triazole ring in the structure of the polymeric compound.

Coordination polymer **1** crystallizes in the P–1 space group with unit cell parameters: *a*=7.2300(5), *b*=10.9685(8), *c*=13.0167(6) Å, α=110.498(5), β=93.266(5), γ=102.508(6)° and features a 3D with a crystal structure in which the tetranuclear cobalt fragment $\{Co_4(OH)_2\}$ and the deprotonated 5-(4-carboxy-5-methyl-1H-1,2,3-triazol-1-yl)isophthalic acid are linked to each other as shown in Figure 1 (a).



a **b**

Figure 1. Crystal structure of $\{[Co_4L_2(H_2O)_2]\cdot 3H_2O\}_n$.

The hydroxyl groups from the isophthalic ring form bridges between the Co1(II) and Co2(II) ions, and a nitrogen atom and an oxygen atom from the carboxyl group of the triazole form a chelate bond with the Co1(II) ion. The experimental magnetic date of **1** have demonstrated that the Co(II) S=3/2 ions are magnetically interacting (Figure 1, b).

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PP1.36

Coordination copper(ii) compounds based on ortho- and para-methoxyphenyl thiosemicarbazones 2-formyl pyridines as inhibitors of cancer cell proliferation

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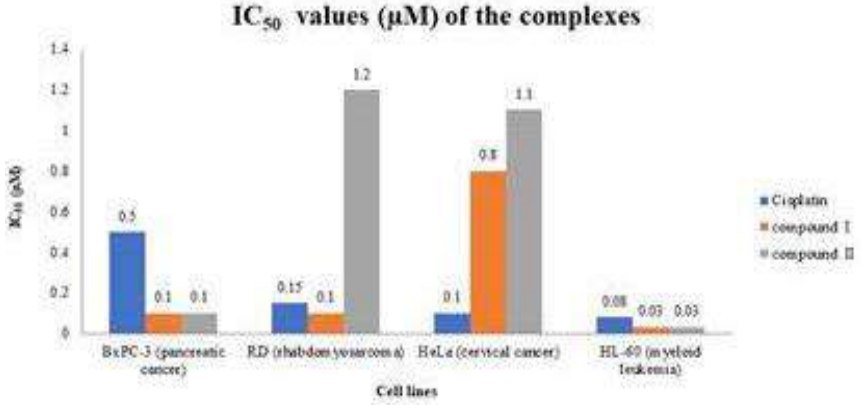
Cancer remains one of the greatest medical challenges, and conventional treatments such as cisplatin, although effective, cause numerous adverse effects (nausea, neuropathy, tachycardia). Recent research aims to identify new, more selective compounds with reduced toxicity [1].

In this research, two new coordination compounds of copper(II) with ligands from the thiosemicarbazone class were studied:$[Cu(L^1)NO_3]$ (**1**) and $[Cu(L^2)NO_3]$ (**2**). These compounds were tested on cancer cell lines (HL-60, HeLa, BxPC-3, RD), using the resazurin method to determine cell viability. The IC_{50} values were compared with those of cisplatin and structural analogues [1-2].



*Name IUPAC compound (**1**) nitrato-{N-[(2-methoxyphenyl)-2-(pyridin-2-yl-methylidene)hydrazine-1-carbothioamido)]}copper(II) and compound (**2**) nitrato-{N-[(4-methoxyphenyl)-2-(pyridin-2-yl-methylidene)hydrazine-1-carbothioamido)]}copper(II).*

The results indicated that our compounds exhibit significant cytostatic activity, surpassing cisplatin by up to 17 times in some cases and being more effective than structural analogues. They represent a promising alternative for the development of innovative anticancer therapies. The copper coordination compounds investigated could expand the therapeutic arsenal against cancer. Through their enhanced biological activity, they can form the basis for the development of more effective cytostatic drugs with reduced adverse effects.

Acknowledgements: This research was funded by the subprograms 010602 and 010701, of the institutional project, Republic of Moldova.

References

1. Rosu, T., et al. Metal-based biologically active agents: Synthesis, characterization, antibacterial and antileukemia activity evaluation of Cu (II), V (IV) and Ni (II) complexes with antipyrine-derived compounds. European Journal of Medicinal Chemistry, 2010, 45.2: 774-781.
2. Rapheal, P. F., et al. Copper (II) complexes of N (4)-substituted thiosemicarbazones derived from pyridine-2-carbaldehyde. Crystal structure of a binuclear complex. Polyhedron, 2007, 26.4: 818-828.

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PP1.37

Novel aminonaphtochinone Mannich bases derived from Lawsone induce cell death on human malignant melanoma cell line A375 by apoptosis and/or necrosis

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Despite significant progress in therapeutic development, cancer is still associated with a major global health issue [1]. As fighting cancer is not trivial, both developing the new therapeutic options, with the emphasis on the efficacious pharmaceutical interventions, and accepting some other treatment modalities including non-pharmaceutical and diagnostic interventions, would allow for more comprehensive, patient-centered management in cancer treatment [2].

Lawsone (2-hydroxy-1,4-naphthoquinone) is one of the remarkable representatives of natural naphthoquinone dyes, for which a broad palette of biological effects is well-documented [3]. Our study was aimed at synthesis and investigation of the antitumor activity of some new lawsone derivatives that were prepared by Mannich reaction, on the basis of described synthetic protocol [4].

Structure elucidation of the synthesized compounds has been performed by using ^{1}H and ^{13}C NMR, IR spectroscopy, GC-MS and elemental analysis.

Human malignant melanoma cell line (A375) was used to test *in vitro* the biological activity of the novel lawsones. Cell culture assays involved MTT and LDH endpoint analyses on a wide range of concentrations (0.5-100 uM), indicating on cell death by apoptosis and/or necrosis in dependence of concentration of compounds. From the biological assays, we can conclude that the tested novel aminonaphtochinone Mannich bases derived from lawsone can be cytotoxic in a concentration-dependent manner, producing oxidative stress and cell death.

Acknowledgements: This research was partially carried out within the project "Chemical study of secondary metabolites from local natural sources and valorization of their applicative potential through the expansion of molecular diversity with multifunctional properties (MetNatVal)" (code: 010601). N.E.D would like to acknowledge the financial support through the "Nucleu" Program within the National Research Development and Innovation Plan 2022–2027, Romania, carried out with the support of MEC, project no. 27N/03.01.2023, component project code PN 23 24 01 02.

References

1. Bray F., Laversanne M., Sung H. et al. CA Cancer J. Clin. 2024; 74(3):229–263 (doi: 10.3322/caac.21834).
2. Cancer research and development landscape: overview of 1999–2022 period. Geneva: World Health Organization; 2024. (doi.10.2471/B09177)
3. Nair A.S., Sekar M., Gan S.H. et al. Drug Des. Devel. Ther. 2024 Jul 26;18:3295-3313. (doi: 10.2147/DDDT.S463545).
4. Neves A.P., Barbosa C.C., Greco, S.J. et al. J. Braz. Chem. Soc. 2009, 20(4): 712-727. (doi: 10.1590/S0103-50532009000400015).

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PP1.38

Synthesis, characterization and biological activity of novel platinum(IV) complexes with fatty acids

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Platinum-based anticancer agents face persistent drawbacks such as systemic toxicity, acquired resistance, and limited molecular selectivity [1]. In this study, new platinum(IV) complexes functionalized with fatty acids—capric, adipic, and palmitic acid—were synthesized and investigated as prodrug candidates.

The platinum(IV) scaffolds were obtained through the oxidation of cisplatin-type precursors, followed by axial coordination of the fatty acid ligands via carboxylate groups. This strategy aimed to enhance lipophilicity, modulate pharmacokinetic properties, and improve intracellular uptake, while retaining the ability of platinum(IV) to undergo reductive activation and release cytotoxic platinum(II) species.

The molecular design was guided by density functional theory (DFT) calculations, which provided structural and electronic predictions prior to synthesis. The structural characterization of the resulting complexes was performed by NMR spectroscopy (^{1}H, ^{13}C, ^{195}Pt), high-resolution mass spectrometry (HRMS), and cyclo-voltammetry to assess the stability and reduction profiles.

These findings demonstrate the potential of fatty acid–functionalized platinum(IV) complexes as dual-action anticancer candidates, where lipophilic axial ligands can enhance delivery and therapeutic efficiency.

Keywords: Pt(IV) prodrugs; fatty acid ligands; lipophilicity; DFT; electrochemistry.

References

1. Neumann, W., Crews, B. C. et al, ChemMedChem. 9, 1150, 2014.

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PP1.39

From platinum to ruthenium: new chemical and clinical frontiers in ovarian cancer treatment

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Introduction. Ovarian cancer is among the most aggressive gynecologic malignancies. Platinum-based drugs, particularly cisplatin and carboplatin, remain the backbone of therapy. Their activity results from covalent binding to guanine bases, inducing DNA crosslinks that block replication and trigger apoptosis. However, resistance mechanisms such as enhanced DNA repair and glutathione detoxification limit efficacy.

Materials and methods. A systematic PubMed search identified ten clinical studies published between 1990–2025. Only studies in patients with epithelial ovarian cancer reporting survival endpoints (PFS, OS) were included. Preclinical reports, animal models, and studies without statistical efficacy data were excluded.

Results. Phase III trials showed similar efficacy for cisplatin and carboplatin (response rates 52–75%, median PFS 14–21 months, OS 32–58 months). Cisplatin was associated with nephrotoxicity and gastrointestinal toxicity, whereas carboplatin induced primarily myelosuppression. The carboplatin–paclitaxel regimen emerged as the standard of care, achieving median OS up to 57 months. Ruthenium complexes (NAMI-A, KP1019/KP1339), investigated only in phase I cohorts, demonstrated plasma stability, albumin binding, and isolated cases of disease stabilization, but no significant objective responses.

Conclusions. Platinum compounds remain the gold standard, with carboplatin offering a more favorable toxicity profile. Ruthenium complexes, through distinct redox chemistry and tumor-selective interactions, represent a promising next-generation approach. Larger phase II/III trials are required to validate clinical benefit and translate chemical innovation into improved patient outcomes.

Keywords: ovarian cancer; cisplatin; carboplatin; ruthenium compounds; resistance; coordination chemistry.

References

1. Clarke MJ. Met Based Drugs. 1999;6:195–211.
2. Allardyce CS, Dyson PJ. Platinum Metals Rev. 2001;45:62–69.
3. Bruijnincx PC, Sadler PJ. Curr Opin Chem Biol. 2008;12:197–206.
4. Swenerton KD, Jeffrey JR. J Clin Oncol. 1992;10(5):718–26.
5. Advanced Ovarian Cancer Trialists 'Group. BMJ. 1991;303:884–93.
6. du Bois A, et al. J Natl Cancer Inst. 2003;95:1320–9.
7. McGuire WP, et al. N Engl J Med. 1996;334:1–6.
8. Ozols RF, et al. J Clin Oncol. 2003;21:3194–200.
9. Rademaker-Lakhai JM, et al. Clin Cancer Res. 2004;10:3715–24.
10. Hartinger CG, et al. Invest New Drugs. 2008;26:217–26.
11. Williams CJ, et al. Eur J Cancer. 1994;30A:1–7.
12. Neijt JP, et al. J Clin Oncol. 2000;18:3084–92.
13. Bookman MA, et al. J Clin Oncol. 2009;27:1419–25.

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PP1.40

Development and characterization of new platinum(IV) complexes with nicotinic acid: synthesis, structural insights, computational studies and electrochemical properties

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Platinum-based chemotherapeutics are limited by systemic toxicity, drug resistance mechanisms, and insufficient selectivity toward cancer cell targets. In this work, novel platinum(IV) complexes incorporating nicotinic acid as axial ligands were synthesized and characterized with the aim of overcoming these limitations [1]. The platinum(IV) scaffolds were obtained via oxidation of cisplatin-type precursors, followed by coordination of nicotinic acid in the axial positions. This functionalization strategy provides multifunctional prodrugs [2] that combine the cytotoxic activity of platinum(II) species released upon intracellular reduction with the pharmacological benefits of nicotinic acid.

The design process was supported by density functional theory (DFT) calculations, which guided the choice of coordination ligands and predicted structural and electronic features relevant for reactivity. The resulting complexes were fully characterized by NMR spectroscopy (^{1}H, ^{13}C, ^{195}Pt), high-resolution mass spectrometry (HRMS), and electrochemical methods, which provided insights into their stability and reduction behaviour.

The incorporation of nicotinic acid into the platinum(IV) framework demonstrates a promising approach toward dual-action anticancer agents, highlighting the potential of rationally designed axial ligands to improve both selectivity and therapeutic efficacy.

Keywords: Pt(IV) prodrugs; nicotinic acid ligands, DFT, electrochemistry.

References

1. Neumann, W., Crews, B. C. et al, ChemMedChem. 9, 1150, 2014.
2. Chen, S., Ng, K. Y. et al, Dalt. Trans.. 51, 885, 2022.

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PP1.41

Experimental research on testing the sensitivity of indicator tubes for the detection of chemical warfare agents

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Global tendencies in researching and developing efficient means of detecting chemical warfare agents constitute a permanent concern for institutes and laboratories, both for specialists working in the national security field, as well as for specialists in other, civilian fields (environmental protection, medicine, mining, chemical synthesis and analysis, refineries, chemical cleaners etc.).

Given the emerging threat to international security, the use of chemical warfare agents (CWAs) represents a major risk both for the armed forces and for the civilian population, and having the capability to rapidly and precisely detect these agents constitutes an essential element for protecting military and civilian personnel.

Indicator tubes are part of the simple chemical detection means, designed for the identification of the main military interest chemical compounds and of the most common toxic industrial compounds (TIC) that can be part of chemical incidents, and are of capital importance in the protection of workers and the general population, and in avoiding the workplace and environmental contamination.

They allow for the detection and identification of substances of interest in vapour or aerosol form in the atmosphere or in enclosed spaces (TI-G for the detection of volatile neurotoxic agents (sarin, soman); TI-ACG gor the detection of phosgene, diphosgene, hydrogen cyanide, cyanogen chloride; TI-HD for the detection of mustard gas; TI-BZ for the detection of BZ psychochemicals; TI-NH_3 for the detection of ammonia; TI-Cl_2 for the detection of chlorine; TI-CO for the detection of carbon monoxide etc.

The indicator tube consists of a glass cylindrical tube, sealed on both ends, that contains an absorbent material impregnated with reactive chemical substances. Upon breaking the tube ends and having the contaminated air run through the tube, the toxic agents react with the reactive chemical substances inside, generating a colour change characteristic of CWAs and/or of the used impregnated substrate (colorimetric detection).

The experimental research has consisted of testing the protection limits of the indicator tubes to specific air toxic substances. The investigations were conducted under normal laboratory conditions (temperature of 22 °C, relative humidity of 68%), by specialized personnel, aughorised to handle CWAs.

Figure 1. Indicator tubes for the detection of CWAs developed through CCIACBRNE.

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PP1.42

Design, synthesis, and characterization of novel pyrrole–terpenic hybrids

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Terpenes are a large and diverse class of naturally occurring organic compounds, widely distributed in plants and known for their structural variety and biological activities. Among them, diterpenes have attracted particular interest due to their potential pharmacological properties. Sclareol, a labdane-type diterpene isolated mainly from *Salvia sclarea* (clary sage), is notable for its antimicrobial, anti-inflammatory, and anticancer activities. Its rigid bicyclic skeleton and reactive functional groups make it a valuable starting material for the synthesis of novel derivatives. Chemical modifications of sclareol, such as functionalization at its hydroxyl groups or transformations of the decalin core, have led to a variety of bioactive compounds, positioning sclareol derivatives as promising scaffolds in medicinal chemistry.

Pyrrol-2-one is a five-membered heterocyclic compound containing both a nitrogen atom and a carbonyl group, which confer significant versatility in synthetic and medicinal chemistry. Its structure serves as a key pharmacophore found in numerous natural products and bioactive molecules, often associated with antimicrobial, anticancer, and anti-inflammatory properties. The lactam functionality within pyrrol-2-one allows for diverse chemical modifications, making it an attractive scaffold for the design of new hybrid molecules. Because of its structural adaptability and biological relevance, pyrrol-2-one derivatives continue to be extensively explored as potential leads in drug discovery and development.

The combination of terpenic frameworks such as sclareol with heterocyclic motifs like pyrrol-2-one represents a powerful strategy for the development of hybrid molecules with enhanced biological activity. Thus, by merging chirality, structural rigidity and functional diversity of terpenes with the pharmacophoric properties of pyrrol-2-one, we present in the current work novel compounds that may exhibit synergistic effects or improved pharmacokinetic profiles. This establishes a foundation for the elaboration of new synthetic targets inspired by natural compounds to address current challenges in drug discovery.

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PP1.43

Synthesis of copper(II) coordination compounds with sulfanilamides and thiosemicarbonazone 2,4-dihydroxybenzaldehyde with antioxidative activity

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Mixed-ligand coordination compounds containing in its composition biologically active aldehyde or ketone and ligand, which is a medicine are of great interest today. Such coordination compounds have been referred to in the literature as pharmaceuticals. Substances with antimicrobial, antifungal, antiviral, anticancer and other biological activities were identified among these compounds [1].

Synthesized 12 mixed-ligand copper(II) coordination compounds containing thiosemicarbazone (H_2L^1) or 4-phenyl-3-thiosemicarbazones (H_2L^2), 2,4-dihydroxybenzaldehyde (H_2L^{1-2}), and sulfonamides such as streptocide (Sf^1), sulfafate (Sf^2), sulfazosol (Sf^3), ethanol (Sf^4), sulfazine (Sf^5), and sulfadimesin (Sf^6), for which the elemental analysis has established the composition $[Cu(Sf)^{1-6}L^{1-2}] \cdot nH_2O$, where n=2-4. The substances were studied by elemental analysis on metal, water, and IR spectroscopy. It was found that the H_2L^{1-2} thiosemicarazones obtained on the copper ion matrix in the composition of coordination compounds behave as tridentate, double-protonated ligands, joining to the central atom through a phenolic oxygen atom from position 2, nitromethane nitrogen, and the thiol atom of sulfur in a deprotonated thiol form, forming five and six membered metal cycles.

The studied sulphanilamides in the composition of complexes behave like monodenate ligands, coordinated to the central atom through the amino group nitrogen atom in the case of streptocide (Str) and sulfazile (Sfc), thiazole or thiodiazole in the case of norsulfate and ethanol, and pyridine nitrogen in the case of sulfazine and sulfadimesin.A study of antioxidant properties indicated that the source substances do not show antioxidant activity (half-peak inhibitory concentration (IC_{50}) is at 58.85 > 100 μM), at that time, as complex compounds exhibit antioxidant activity in the range of inhibition concentrations from 3.45 to 63.03 μM. The inhibitory concentration (IC_{50}) of the synthesized coordination compounds depends primarily on the nature of the sulfanilamide and varies in the series Etz > Str > Sfz > Sfc > Nor > Sfdz. Coordination compounds with ethazole and streptocide for antioxidant activity are more active than Trolox, used in medicine as a reference, and complexes with other sulfanilamides are inferior in activity.

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References

1. Graur, V., Gulea, A. Novel biological agents based on metal complexes of N4-allylthiosemicarbazones and their derivatives. Monograph. Chișinău: CEP USM, 2024, 290 p. ISBN 978-9975-62-716-0.

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PP1.44

The biological relevance of Pt(IV) prodrugs with specific axial ligands

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Bifunctional assemblies featuring an organic ligand with therapeutic potential coordinated to a cisplatin-like Pt(IV) framework can act as prodrugs, as the cellular environment reduces platinum(IV) to platinum(II), thus liberating in situ cisplatin (or variations thereof) and the additional drug. Studying the interactions of potential drugs with proteins provides us with information regarding mechanisms of action, side effects and selectivity [1].

The research presented here explores the behavior of Pt(IV) complexes in biologically relevant interactions with the aim of developing new selective anticancer drugs. Ligands such as fenbufen, benoxaprofen, ibuprofen, oxaprozin, nicotinic acid and capric acid were used for coordination.

The above- mentioned interactions were monitored using spectroscopy UV-Vis and fluorescence. A major component of blood, to which any therapeutic agent would be exposed, is hemoglobin (Hb). A range of compounds with therapeutic action/potential (anticancer and beyond), including Pt(II)-based compounds, have been shown to affect the oxidative reactivity of Hb – either by acting as antioxidants or as agents of oxidative stress that promote Hb autoxidation [2]. Thus, the oxy-Hb autoxidation reaction was studied, in the presence of Pt(IV) hexacoordinated complexes and also of ligands. The peroxidase reactivity of Pt(IV) complexes and ligands was assayed with ferryl-Hb. Binding of complexes to albumin as well as to Hb was confirmed by fluorescence measurements.

DNA binding was also studied by fluorescence assays for the same set of compounds. As expected, the ligands do not bind to DNA, while all Pt(IV) complexes do. We have identified compounds with high affinity for DNA, which suggests potential biomedical applications for the development of new cytostatic treatments.

Pt(IV) drug candidates are generally expected to be reduced to Pt(II) by thiol pools inside living cells[1], so the reaction between glutathione (GSH) and Pt(IV) complexes was spectrophotometrically followed. A decrease in absorbance was found, indicating reduction to Pt(II) – as also confirmed by TD-DFT calculations.

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References

1. Richter S., Lonnecke P., Bovan D., Andrian N., Stoean B., Lehene M., Silaghi-Dumitrescu R., Gaina L., Mijatovic S., Maksimovic-Ivanic D., Kaluderovic G.N., Hey-Hawkins E., Dalton Trans., 2025, 54, 3597.
2. Zagrean-Turza C., Igescu I., Lupan A., Silaghi-Dumitrescu R., Inorg. Chim. Acta, 2024, 567, 122053.

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PP1.45

Antioxidant properties of coordination compounds of Cu(II) and Bi(III) with aminopolycarboxylate and 2-formylpyridine 4-phenylthiosemicarbazone ligands

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The research is focused on the synthesis and characterization of seven homometallic and heterometallic coordination compounds of Copper(II) and Bismuth(III) with some aminopolycarboxylate (ethylenediaminetetraacetate - $edta^{4-}$; 1,2-cyclohexanediaminetetra-acetate - $cdta^{4-}$; diethylenetriaminepentaacetate - $dtpa^{5-}$) and 2-formylpyridine 4-phenyl-thiosemicarbazone mixed-ligands. The interest in this class of compounds arose from the crucial role of free radicals in biological processes, ranging from anti-aging to various pathologies. Substances capable of neutralizing these radicals, known as antioxidants, are of considerable importance in the medical realm.

The antioxidant properties of the synthesized compounds have been evaluated by determining the half-maximal inhibitory concentration (IC_{50}), using the $ABTS^{+}$ free radical scavenging method. The results demonstrated that five of seven complexes exhibited remarkable antioxidant activity, with IC_{50} values ranging from 2.47 to 13.08 μM. These values are significantly superior to those of Trolox, a reference antioxidant, which IC_{50} value is 15.86 μM, the antioxidant property of the obtained coordination compounds being 1.21 to 6.42 times higher than that of Trolox. The most effective was found to be the complex of Bi(III) with 2-formylpyridine 4-phenylthiosemicarbazone and $edta^{4-}$ anion, which IC_{50} value is 2.47 μM. This value is approximately 3.76 times greater than that of the non-coordinated thiosemicarbazone and 6.42 times higher than the one of Trolox. These findings suggest that the coordination of organic compounds to metallic ions can significantly enhance the antioxidant properties of the ligands, opening new perspectives for the design of metallo-organic compounds with therapeutic potential.

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PP1.46

Personal kit for immediate decontamination

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The proliferation of chemical, biological, radiological and nuclear weapons (CBRN) constitute a direct military threat to the population, territory and allied forces, representing a serious concern for the Alliance.

Along with gas mask, the individual package for immediate decontamination is a necessary component that all soldiers that are in combat missions or civilian personnel of intervention teams must equip.

In the case of terrorist incidents such as CBRN or military actions with the use of weapons of mass destruction, the individual decontamination is an extremely urgent measure for the rescue of personnel from all categories of military forces or specialized intervention teams, and the unprotected civilian population. Any delay has a significant impact on the performance of combat missions, volume loss and recovery success.

This paper presents a kit for the individual protection and immediate decontamination of the personnel (TIDI), within a very short time, guaranteeing the chances of survival. The product was realized according with the NATO required standards.

TIDI is intended for military personnel from all military forces and provides chemical, biological and radiological decontamination of the body, equipment, weapons and materials which are in the possession of military personnel.

The product is based on an amino alcoholic solution with a multiple decontamination effects, impregnated on an inert chemically support, used both for skin and affected portions of equipment and weapons decontamination.

Figure 1. Personal kit for immediate decontamination (TIDI) developed through STIMPEX SA.

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References

1. AEP 58 - Operational features, technical specification, tests procedures and assessment criteria for CBRN defence equipment.

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PP1.47

Copper(II) complex with a redox-noninnocent Schiff base: synthesis, structure and catalytic oxidation of cyclohexane

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We present an organic-inorganic diamine, 1,3-bis(aminopropyl)tetraphenyldisiloxane was prepared and introduced as a flexible spacer in the structure of a salen-type Schiff base (**H_2L^7**) extending the available small library of similar compounds derived from 1,3-bis(aminopropyl)tetramethyldisiloxane and substituted 2-hydroxybenzaldehydes (**H_2L^1**–**H_2L^6**). Like previously reported mononuclear copper(II) complexes **[CuL^1] –[CuL^6]**, the new copper(II) complex **[CuL^7]**, obtained by reaction of $Cu(OAc)_2 \cdot H_2O$ with **H_2L^7** in a mixture of organic solvents, has a tetrahedrally distorted square-planar (N_2O_2) coordination geometry. X-ray crystallography has shown that compared to **[CuL^1] –[CuL^6]** the Si–O–Si angle in **[CuL^7]** is even closer to linear due to stronger intramolecular interactions between Ph groups than between Me groups in the central $–R_2Si–O–SiR_2–$ fragment (R = Ph and Me, respectively). **[CuL^7]** can be electrochemically reversibly oxidized by two successive one-electron processes generating a stable phenoxyl mono- and diradicals. Both oxidations are ligand-centered leading to the formation of coordinated phenoxyl radicals. The UV spectrum of **[CuL^7]** consists of $\pi \rightarrow \pi^*$ and LMCT $\sigma \rightarrow$ d transitions. The low-energy d-d absorption is well described by AILFT CAS(9,5)/NEVPT2 calculations. The one-electron oxidized compound **[CuL^7]$^+$** should exist in the triplet ground state as **^{3}[CuL^7]$^+$** with the two unpaired electrons located on d_{x2-y2} orbital of copper(II) (d^9, $S_{Cu} = ½$) and the molecular orbital (MO) comprising p_z oxygen and carbon atoms of the phenoxyl radical ($S_{rad} = ½$). The broad absorption in the vis-NIR region of the optical spectrum of the one-electron oxidized complex is due to $\pi \rightarrow \pi^*$ transitions in triplet species **^{3}[CuL^7]$^+$**, but not in **[CuL^7]$^{2+}$** one. The doubly oxidized **[CuL^7]** species shows very close doublet and quartet states, where the doublet state has an unpaired electron located on the Cu(II) d-orbital, while π-bonding orbitals contain an electron pair forming a multireference state. In all state-averaged CASSCF cases the occupation of the Cu(II) d-orbital is nearly 1.0, indicating its limited involvement into the excited states. Catalytic studies showed that **[CuL^7]** acts as a catalyst of oxidation of alkanes with peroxides under very unusual solvent-free conditions, converting cyclohexane into cyclohexanol and cyclohexanone (with hydrogen peroxide or *tert*-butyl hydroperoxide as oxidant) or into cyclohexanol and *ε*-caprolactone (with *m*-chloroperoxybenzoic acid as oxidant.

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PP1.48

Reactivity of vitamin B_{12} and related compounds with small molecules

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Vitamin B_{12} (cobalamin, Cbl) plays essential biological roles, yet its reactivity toward biologically relevant oxidants remains insufficiently explored compared to related metallomacrocycles such as hemes. This work investigates the chemical reactivity of cobalamin with small oxidant molecules, including hydrogen peroxide, hypochlorite, chlorite, and m-chloroperoxybenzoic acid (mCPBA).

For the first time, we describe a stable and reversible Co(III)–hydroperoxide adduct, formed upon binding of deprotonated H_2O_2 in a monodentate fashion. The initial outer-sphere oxidation of Cbl(II) by H_2O_2 generates Cbl(III) and hydroxyl radicals, which may either attack the corrin ring, producing side products, or diffuse into solution, leaving intact Co(III). With mCPBA, Cbl(III) forms a peroxoacid complex, demonstrating that peroxide coordination chemistry of cobalamin extends beyond hydrogen peroxide, although not all peroxo species bind effectively.

Reactions with hypochlorite revealed transient intermediates; for CNCbl, evidence supports a ClO–Co(III)–CN adduct formed by benzimidazole substitution. In contrast, chlorite yields a stable Co(III)–chlorite complex, markedly different from ferric hemes, where O–Cl bond cleavage occurs within microseconds.

These findings expand the known oxidative coordination chemistry of vitamin B_{12} and highlight key differences from heme reactivity, providing insights into the unique roles of cobalamin in redox biology.

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PP1.49

Spectroscopic evaluation of the interaction of Myoglobin with biomedically relevant compounds

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This study investigates the redox behavior of myoglobin (Mb) in the presence of several bioactive compounds with biomedical relevance. These include the well-known Pt(II) drug, cisplatin, oxoplatin (a Pt(IV) compound representative for a newer-generation drugs based on platinum), capric acid, fenbufen, plumbagin and fisetin. These molecules were selected based on their structural diversity and documented biological effects, such as anti-inflammatory, chemotherapeutic, or antioxidant properties. The study aimed to evaluate how these compounds affect the structural and redox properties of Mb, particularly in terms of their capacity to bind to the protein and modulate its oxidation state.

Spectroscopic methods (UV-Vis absorption, fluorescence, and NMR) and docking calculations were used to monitor binding and modifications of the redox state of the Mb in reactions such as autoxidation, nitrite-induced autoxidation, and peroxide-induced damage. These experiments are designed to parallel previous findings with similar experiments on hemoglobin with small molecules of biomedical/therapeutic relevance [1–4]. Our results demonstrate a differential response: while some compounds induced minimal or no spectral changes - suggesting limited interaction or redox impact, while others, such as fisetin and plumbagin, displayed notable pro-oxidative effects.

These findings suggest that fisetin and plumbagin may act as pro-oxidants or interact with Mb through mechanisms that alter their redox state, while the other compounds may exhibit stabilizing or potentially antioxidant effects. The observed variability highlights the complex nature of small molecule-protein interactions and underlines the importance of assessing individual compound behavior in biochemical systems.

This work contributes to a better understanding of how diverse small molecules influence the redox chemistry of globins, with implications for pharmacology and redox biology.

References

1. S. Richter; P. Lönnecke; D. Bovan; N. Andrian; B. Stoean; M. Lehene; R. Silaghi-Dumitrescu; L. Gaina; S. Mijatović; D. Maksimović-Ivanić; G. N. Kaluđerović; E. Hey-Hawkins; Dalton Trans. 2025, 54, 3597–3609.
2. C. Puscas; A. Mircea; M. Raiu; M. Mic; A. A. A. Attia; R. Silaghi-Dumitrescu; Chem. Res. Toxicol. 2019, 32, 1402–1411.
3. C. Zagrean-Tuza; I. Igescu; A. Lupan; R. Silaghi-Dumitrescu; Inorg. Chim. Acta 2024, 567, 122053.
4. C. Zăgrean-Tuza; A. Matei; R. Silaghi-Dumitrescu; J. Inorg. Biochem. 2024, 112613. doi:10.1016/J.JINORGBIO.2024.112613

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PP1.50

Preparation of cinchonine-carboxylic acid co-crystals through a charge-assisted hydrogen bonding assembly process

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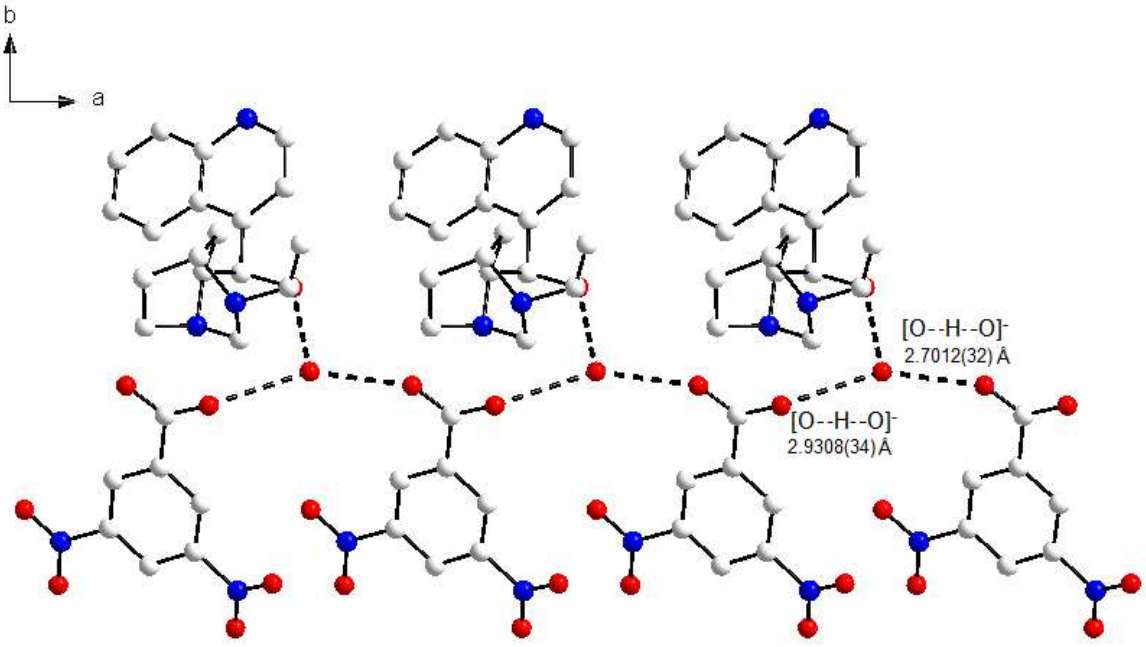
Hydrogen bonding is one the most widely used interactions to generate supramolecular systems with a variety of novel structural features, unique chemical and physical properties. As supramolecular H-bonding synthons, carboxylate compounds have been widely used to construct organic functional solids due to their excellent H-bonding capability, leading to expanded structures or open metal-organic frameworks.

In this work, we discuss the co-crystallization of cinchonine with various carboxylic acids (e.g. oxalic acid and 3,5-dinitrobenzoic acid) through a charge-assisted hydrogen bonding (CAHB) self-assembly process as a useful tool for designing crystalline solids. X-ray diffraction, FTIR and NMR spectroscopy were performed to elucidate the structures of the cinchonine-carboxylic acids co-crystals formed under different crystallization parameters (pH, temperature, solvent).



Fragment of the crystal structure of cinchonine·3,5-dinitrobenzoate.

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PP1.51

Japanese pagoda tree (*Sophora japonica* L.) growing in Moldova as a source of bio-organic compounds

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Japanese pagoda tree (*Sophora japonica* L., syn. *Styphnolobium japonicum* (L.) Schott) is one of the oldest medicinal plants used in traditional medicine. The species, originating from China, is currently widespread in Europe, including the Republic of Moldova as an ornamental tree, but is especially recommended for the creation and rehabilitation of protective forest curtains [1-3]. The species is a valuable melliferous with a late flowering period [4], and the flowers, flower buds and extracts from them are used in the production of cakes, drinks and as preservatives in sausages [5-7]. The main uses of immature flower buds, flowers and fruits remain in medicine, however, due to the cardiovascular, anti-inflammatory, anti-osteoporotic, antioxidant, antitumor, antibacterial, antiviral, hemostatic and anti-atherosclerotic effects. that they exhibit. In the specialized literature, there are only a few mentions of the chemical composition of the volatile oil obtained from *S. japonica* flowers and the fatty oil from the seeds [8,9], and data referring to the population of the Republic of Moldova are completely missing.

Samples of essential oil from flowers and fatty oil from seeds of S. japonica of Moldovan origin were analyzed using GC-MS method. About 59 constituents of the volatile oil were identified, the major compound being carvacrol (25.4%), followed by linalool (19.2%), linalyl acetate (10.7%) and thymol (6.4%). The chemical composition of the fatty oil is determined by *n*-docosanoic (C22:0, 21.3%), *p*-methoxy-2-propenoic (C4:0, 11.5%), *n*-eicosanoic (C20:0, 19.3%) and *n*-tetracosanoic (C24:0, 6.3%) acids.

According to experimental data, the Moldovan population of *S. japonica* is a valuable source of biologically active compounds for the pharmaceutical industry.

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References

1. Yu J., Xu L.-R., Liu C., Li Y.-T., Pang X.-B., Liu Z.-H., Yang M.-S., Li Y.-H. Comparative analysis of the dust retention capacity and leaf microstructure of 11 *Sophora japonica* clones. PLoS ONE, 2021, 16(9), e0254627. DOI: https://doi.org/10.1371/journal.pone.0254627
2. Galupa D.; Talmaci, I. Înființarea perdelelor forestiere de protecție în calitate de măsură de adaptare la schimbările climatice: Ghid practice pentru producătorii agricoli. Uniunea Consolidată pentru Implementarea Programelor IFAD (UCIP IFAD). Chișinău: Bons Offices, 2021, 60 p. ISBN 978–9975–87–683–4
3. Лось С.А., Терещенко Л.І., Бойко Н.М. Стіфнолобіум японський (S*tiphnolobium japonicum* (L.) Schott.) На території дсдлц «веселі боковеньки». «Наукові читання імені В.М. Виноградова»: Матеріали VII-ої Всеукраїнської науково-практичної конференції. 8–9 травня 2025 року. Херсон Кропивницький: 2025. 178 с. DOI: 10.32782/895-2025-nature-conf
4. Nikolova T., Petrova A., Yordanova A. Study of the honey productivity of some tree species. Scientific Papers, 2018, 61(2), pp. 216-219. ISSN 2285-5750. ISSN Online 2393-2260. ISSN-L 2285-5750.
5. Li Y., Fan L. Comparative studies on the stabilization of *Flos sophorae immaturus* beverages by various hydrocolloids. LWT-Food science and technology, 2020, 123, 109117. DOI: https://doi.org/10.1016/j.lwt.2020.109117
6. Hong S.F., Yun L.L., Hong S.X., Jun T., Rui W.J., Gang, C. Optimization of stir-baked technology for *Flos sophorae immaturus* tea according to quadratic regression rotation-orthogonal design method and quality evaluation. Italian Journal of Food Science, 2021, 33(1), 84–95. DOI: https://doi.org/10.15586/IJFS.V33I1.1977
7. Tang R., Peng J., Chen L., Liu D., Wang W., Guo X. Combination of *Flos sophorae* and chili pepper as a nitrite alternative improves the antioxidant, microbial communities and quality traits in Chinese sausages. Food Research International, 2021, 141, 110131. DOI: https://doi.org/10.1016/j.foodres.2021.110131
8. Mahmoud Abudayeh Z.H.,, Khaldun M. Al Azzam K.M., Cholak I.S., Uliana Vladimirovna Karpiuk U.V., Naddaf A., Aboul-Enein H.Y. Analysis of essential oil in *Sophora japonica* L. flower buds on different stages of development by gas chromatography-mass spectrometry. World Journal of Analytical Chemistry, 2015, 3(1A), 15-20.
9. Olennikov D.N, Tankhaeva L.M., Sandanov D.V. Fatty acids from seeds of *Sophora flavescens* and *Styphnolobium japonicum*. Chemistry of Natural Compounds, 2009, 45(2), 225-226.

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PP1.52

Characterization of some metal phthalocyanines using transient absorption spectroscopy

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In this work, the nanosecond and femtosecond transient absorption techniques were applied to study the photophysical properties of some new compounds such as phthalocyanine derivatives and metal complexes. For this purpose, synthesized compounds present excellent emission properties and stability. We choose the investigation for the theoretical information and applications resulting from this study, to develop new technological innovations for the health sciences with applications in medicine.

In order to demonstrate the excited-state processes from the transient absorption map, we obtained a ground state bleaching band (**GBS**), absorption in excited state (**ESA**) and at longer wavelength stimulated emission (**SE**). Also, lifetime as well as the fluorescence emission, and quantum yield are typical and important spectroscopic parameters of the singlet state, which depends on the interaction of the molecule with its environment, leading to useful information about this interaction. The knowledge of excited- state absorption is important in the design of fluorophores for the biological and medical applications, because it may reduce their brightness, thereby limiting their potential in application. The understanding of the photoproperties is overall crucial in the design of the organic fluorophores.

Keywords: transient absorption spectroscopy, phthalocyanine derivatives.

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PP1.53

Structural diversity of sclareol degradation products and their medicinal chemistry potential

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Drug discovery and medicinal chemistry continue to benefit from natural products such as sclareol - a commercially available bicyclic diterpene diol isolated from *Clary sage* (*Salvia sclarea* L.), which serves as a versatile precursor for the generation of structurally diverse bioactive scaffolds [1]. Owing to its distinct molecular architecture, sclareol readily undergoes extensive chemical modification, thereby providing access to a wide spectrum of biologically active derivatives (*figure 1*). Presence of reactive functional groups imparts selective reactivity, facilitating transformations on both the lateral prenylated chain and the *trans*-decalin core. We present in the current communication the synthetic pathways to an array of sclareol-derived products with different structural features. These features collectively enable fine-tuning of structure-activity relationships, making sclareol an attractive scaffold for the design and development of novel anticancer, antifungal, and antibacterial agents.

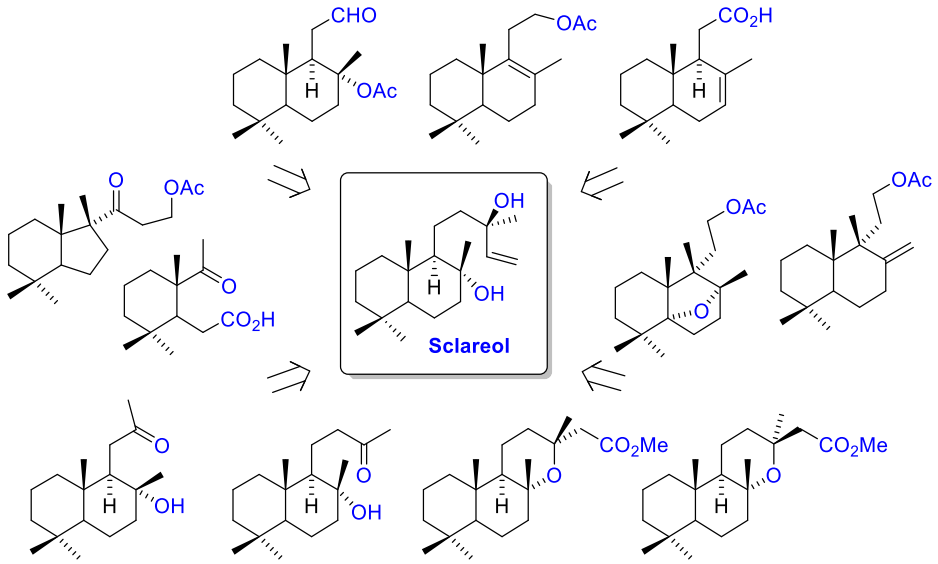

Figure 1. Representative products derived synthetically from sclareol.

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References

1. Selka, A.; Abidli, A.; Schiavo, L.; Jeanmart, L.; Hanquet, G.; Lubell, W. L. European Journal of Organic Chemistry, 2025, 28, e202400983. DOI: https://doi.org/10.1002/ejoc.202400983

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PP2.1

The biochemical pathways that lead to illicit drugs-induced stroke

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Stroke is a neurological disorder that implies brain ischaemia with rapidly evolving clinical signs or focal neurological deficits that persist for more than 24 hours. In contrast, a transitory ischaemic attack (TIA) resolves within 24 hours. A narrative literature review was conducted to explore the relationship between illicit drug use and stroke pathogenesis. Illicit drugs are known to induce stroke *via* various mechanisms. Cocaine, for example, promotes the formation of aminochromes, and generates reactive oxygen species (ROS) through its metabolites [1]. These processes contribute to cardiovascular complications such as cardiomyopathy, vasospasm, and surges in arterial blood pressure, largely due to the upregulation of calcium channels and downregulation of potassium channels. D-amphetamine derivatives, which have pharmacological properties similar to antidepressants, antiparkinsonian agents, or neurotropic drugs, are transported into the neurons of the lateral reticular formation of the brainstem with co-transport with two sodium ions, and a chloride ion. Once internalized, they stimulate the vesicular monoamine transporter type 2 (VMAT-2) promoting the release of monoamine neurotransmitters into the extracellular space. They also inhibit monoamine reuptake and may block monoamine oxidase (MAO), resulting in an accumulation of neurotransmitters at the synaptic cleft. Methylphenidate shares the same mechanism of action, with the exception of MAO inhibition [2]. MDMA (ecstasy) will induce a well-known oxidative/nitrosative stress, generating ROS, and reactive nitrogen species (RNS), including peroxynitrite ($ONOO^-$). This radical may nitrate the tyrosine residues, and S-nitrosylate cysteine residues. Lipid, protein, and mRNA peroxidation have also been reported. Moreover, Janus kinase, and p38 kinase signaling pathways are disrupted, leading to irreversible cellular damage. In heroin users, increased expression of the G protein-coupled receptor kinases (GRK) – GRK2, GRK6 and β-arrestin-2 has been observed in the prefrontal cortex, along with signs of hippocampal neuronal lesions proven by elevated glial fibrillary acid protein (GFAP) [3]. Phencyclidine (PCP) exhibits a high affinity for NDMA receptors in the hippocampus, neocortex, basal ganglia, and limbic system. It also shows a moderate affinity for the reuptake systems of norepinephrine, dopamine, and serotonin along with the opioid receptors. PCP stimulates tyrosine hydroxylase, increasing norepinephrine and dopamine synthesis and enhances glutamate release by inhibiting glutamate-sensible receptors. The molecular mechanisms of lysergic acid diethylamide (LSD) are less well understood. However, it has been proven that mainly the HT_{1A} receptor along with 5-HT_1 subtypes 5-HT_{1B}, 5-HT_{1D}, and 5-HT_{1E} may be activated by this illicit drug. Effects of LSD on 5-HT_{2C}, 5-HT_{5A}, 5-HT_6, and 5-HT_7 are uncertain. Endocannabinoids activate the CB1, and CB2 receptors both coupled to inhibitory G-proteins. Activation of these receptors can reduce the expression of pro-inflammatory cytokines, potentially contributing to stroke-related pathophysiology [4]. Cannabis may inhibit the I, II, and III complexes of the electron transport chain, resulting in mitochondrial uncoupling and increased ROS production [5]. In conclusion, illicit drugs exert complex, multifactorial effects on cerebrovascular health, involving both known and poorly elucidated molecular pathways. These effects are often dose-dependent and influenced by genetic predisposition and comorbidities, making them unpredictable and clinically significant in the context of stroke risk.

References

1. Liaudet L, Calderari B, Pacher P. Pathophysiological mechanisms of catecholamine and cocaine-mediated cardiotoxicity. Heart Fail Rev 2014;19(6):815-24. doi: 10.1007/s10741-014-9418-y.
2. Ferreira M, Carneiro P, Costa VM, et al. Amphetamine and methylphenidate potential on the recovery from stroke and traumatic brain injury: a review. Rev Neurosci. 2024;10;35(7):709-746. doi: 10.1515/revneuro-2024-0016.
3. Blackwood CA, Cadet JL. The molecular neurobiology and neuropathology of opioid use disorder. Curr Res Neurobiol 2021;2:100023. doi: 10.1016/j.crneur.2021.100023.
4. Carter C, Laviolette L, Bietar B, et al. Cannabis, Cannabinoids, and Stroke: Increased Risk or Potential for Protection-A Narrative Review. Curr Issues Mol Biol 2024;46(4):3122-3133. doi: 10.3390/cimb46040196.
5. Wolff V, Schlagowski AI, Rouyer O, et al. Tetrahydrocannabinol induces brain mitochondrial respiratory chain dysfunction and increases oxidative stress: a potential mechanism involved in cannabis-related stroke. Biomed Res Int 2015;2015:323706. doi: 10.1155/2015/323706.

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PP2.2

Curcuma longa extracts optimized for wound care: antioxidant, antimicrobial, antibiofilm, anti-inflammatory and selective cytotoxic activity

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Curcuma longa L., long recognized for its pharmacological potential, has been intensively studied for its rich content in curcuminoids and essential oils [1,2,3]. This study' objective was to optimize extraction strategies capable of attenuating oxidative stress while delivering broad-spectrum antimicrobial activity relevant to tissue lesions in infected wounds.

Five hydroalcoholic extracts (T0-T4) were prepared by combining dynamic maceration (DM), enzymatic extraction (cellulase, EE), and ultrasound-assisted extraction (UAE), then characterized spectrophotometrically for total polyphenols and flavonoids and individual components by UHPLC-MS/MS. The antimicrobial properties were assessed against 15 reference and clinical isolates, using qualitative (adapted diffusion) and quantitative (broth microdilution) methods. The antibiofilm activity on an inert substrate was determined by quantifying the biofilm mass using a colorimetric assay and by evaluating the biofilm metabolic activity using the MTT assay. Antioxidant capacity was profiled by DPPH, TEAC, CUPRAC, and FRAP assays with nitric-oxide scavenging measured to infer anti-inflammatory potential. Finally, biocompatibility on HaCaT keratinocytes together with cytotoxicity on A-431 epidermoid carcinoma cells were evaluated using MTT and LDH-release for the extract showing the best antimicrobial–antioxidant profile.

Among the *C. longa* variants, EE performed in citrate buffer and coupled to UAE and DM achieved the highest yield (3.86 ± 0.15% of rhizome dry weight; T2), whereas the extract with the greatest polyphenolic load was obtained by EE in water subsequently adjusted to 50% ethanol, followed by 10 min UAE and 48 h DM (T3), and the extract richest in flavonoids resulted from UAE plus DM (T4); UHPLC-MS/MS identified phenolics including curcumin, *p*-coumaric acid, isorhamnetin, and 4-hydroxybenzoic acid. Antioxidant activity varied significantly with extraction conditions, with the lowest IC_{50} values recorded for T4, while CUPRAC, TEAC, and FRAP corroborated marked differences in reducing capacity. Notably, T3 exhibited the strongest NO-scavenging at 2.5 mg dry extract/mL (82.69 ± 6.38%). The extracts displayed broad-spectrum antibacterial activity with MICs of 0.156–5 mg/mL against *Staphylococcus aureus*, *Enterococcus faecalis*, and *Pseudomonas aeruginosa* isolated from infected wounds, as well as activity against the microfungal strain *Candida parapsilosis*. Adhesion to inert substrata was reduced across strains, with T3 providing the most consistent antibacterial and antibiofilm effects, alongside selective cytotoxicity favoring tumor over normal cells.

Collectively, these findings indicate that careful optimization of the extraction technique is pivotal for generating *C. longa* extracts with superior antioxidant and antimicrobial properties, underscoring their relevance as candidate adjuvants in the development of effective interventions for infected wounds.

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References

1. https://doi.org/10.3390/ijms20051119,
2. https://doi.org/10.3390/ijms25073617,
3. https://doi.org/10.22159/ijap.2024.v16s1.33.

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PP2.3

Biochemical interactions of the gut-brain-axis in the first 1000 days of child development

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Background. In the first 1000 days, intestinal bacteria produce a wide range of biochemical mediators that influence brain plasticity. The gut–brain axis represents a bidirectional communication network between the central nervous system and the digestive system, supported by neuronal, endocrine, immune, and metabolic mediators, playing an essential role in maintaining the body's homeostasis.

Objective of the study: to synthesize the biochemical interactions between the intestinal microbiome and the central nervous system in the early years of life, based on the most recent scientific evidence.

Material and methods. A narrative and integrative analysis of the scientific literature from major databases such as PubMed, Research4Life, Web of Science (2020–2025), which included articles on microbial mediators of the gut–brain axis in children during the first 1000 days of life, with a focus on clinical studies, systematic reviews, and meta-analyses.

Results. This analysis identified the existence of more than 20 biochemical mediators through which the intestinal microbiome influences the neurological development of children in early childhood. The most frequently studied are: short-chain fatty acids, serotonin, gamma-aminobutyric acid, dopamine, acetylcholine, histamine, as well as pro-inflammatory cytokines and tryptophan metabolites (e.g., kynurenine, indoles). In addition, emerging mediators were identified, such as microbiota-regulated microRNAs, secondary bile acid metabolites, bacterial polyamines, phenolic compounds, extracellular vesicles, and endogenous neurosteroids, suggesting an extended network of bidirectional interactions between the gut and the central nervous system.

Conclusions. Early childhood represents a critical window for child development, during which the intestinal microbiome influences the gut–brain axis through a variety of biochemical messengers. A comprehensive understanding of the composition of the intestinal microbiome and the mechanisms involved in gut–brain interactions could open new therapeutic perspectives for neurodevelopmental disorders in children.

Keywords: Gut–Brain Axis; Intestinal Microbiome; Developmental Disorders; Children 0–3 years.

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PP2.4

Immunogenetic associations in axial involvement of juvenile idiopathic arthritis: a meta-analysis

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Background. Axial involvement in juvenile idiopathic arthritis (JIA), characterized by inflammation of the spine and sacroiliac joints, is a significant clinical manifestation that can lead to long-term disability. The pathogenesis of axial JIA is complex, involving genetic predispositions and immune system dysregulation. Human leukocyte antigen B27 (HLA-B27) has been implicated in the development of spondyloarthropathies, including axial JIA. Additionally, pro-inflammatory cytokines such as IL-17, IL-23, and TNF-α play pivotal roles in the inflammatory processes associated with axial involvement.

Objective: to systematically evaluate and synthesize the available evidence on the immunogenetic factors, specifically HLA-B27, and the serum levels of pro-inflammatory cytokines IL-17, IL-23, and TNF-α in pediatric patients with axial JIA.

Methods. A comprehensive literature search was conducted across multiple databases, including PubMed, Scopus, and Web of Science, for studies published up to 2025. Studies were included if they reported on the prevalence of HLA-B27 and serum levels of IL-17, IL-23, and TNF-α in children diagnosed with axial JIA. Data were extracted on study characteristics, sample sizes, HLA-B27 prevalence, and cytokine levels. Pooled estimates were calculated using random-effects models, and heterogeneity was assessed using the I^2 statistic.

Results. Preliminary findings suggest a significant association between HLA-B27 positivity and increased serum levels of IL-17, IL-23, and TNF-α in children with axial JIA. The pooled prevalence of HLA-B27 in this population was estimated to be approximately 60%, with higher levels of the aforementioned cytokines observed in HLA-B27-positive individuals compared to HLA-B27-negative counterparts. These findings align with the known pathophysiological role of the IL-23/IL-17 axis in spondyloarthritis and support the hypothesis that HLA-B27 may influence cytokine production, thereby contributing to disease pathogenesis.

Conclusion. This meta-analysis underscores the significant role of HLA-B27 and pro-inflammatory cytokines in the immunopathogenesis of axial JIA. The findings highlight the potential for targeting the IL-23/IL-17 axis in therapeutic strategies for this condition. Further well-designed, multicenter studies are needed to confirm these associations and explore their clinical implications.

Keywords: Enthesitis-related arthritis, HLA-B27, IL-17, IL-23, TNF-α, cytokines, juvenile idiopathic arthritis, pediatric rheumatology.

References

1. Weiss PF, Reiff A, Colbert RA, et al. Enthesitis-related arthritis: a multisite study of 234 patients. Arthritis Res Ther. 2017;19(1):100. doi:10.1186/s13075-017-1297-x.
2. Jittawattanarat R, Wangsiricharoen S, Tangcheewinsirikul N, et al. Clinical characteristics and treatment outcomes in children with enthesitis-related arthritis. Pediatr Rheumatol. 2024;22(1):30. doi:10.1186/s12969-024-00894-2.
3. Ringold S, Angeles-Han ST, Beukelman T, et al. Comparative effectiveness of tumor necrosis factor inhibitors and methotrexate in children with enthesitis-related arthritis. Arthritis Res Ther. 2018;20(1):167. doi:10.1186/s13075-018-1653-0.
4. Zhang X, Huang J, Guo W, Jin P, Yan S, Wang L, et al. Effectiveness of tumor necrosis factor inhibitors in children with enthesitis-related arthritis: a single-center retrospective analysis. Front Pediatr. 2023;11:1163292. doi:10.3389/fped.2023.1163292.
5. Moncrieffe H, Vogl T, Foell D, Holzinger D. The role of interleukin-17 in juvenile idiopathic arthritis: from pathogenesis to treatment. Int. J. Mol. Sci., 2022;23(24):15603. doi:10.3390/ijms232415603.

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PP2.5

The choice of the optimal composition of hard capsules with Dioxoindolinone

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Bioavailability of medicinal substances is one of the relevant criteria for evaluating the therapeutical efficiency of the drug during the developing process of its technology and composition. It is necessary to study the biopharmaceutical properties, especially of the pharmaceutical forms with systemic administration, where the speed and degree of the absorbtion influence directly its bioavailability and efficiency. The process of dissolving an active substance in the gastrointestinal tract is simulated by the "dissolving" test in vitro, which is characterized by the pharmaceutical availability of the drug and serves as an important factor in choosing the optimal composition and technology. Dioxoindolinone (DIOX) is a local product synthesized in the Organic Synthesis laboratory of the Institute of chemistry, and shows an important pharmacological potential for the treatment of NCS diseases. According to the previous data, the goal of this paper is to study the influence of pharmaceutical factors on the release process of DIOX from the pharmaceutical form, in order to select the optimal composition of capped capsules. The study object was DIOX and excipients (EX): microcrystalline cellulose (CMC), sodium starch glycolate (AGNa), polyvinylpyrrolidone (PVP) K30 (HIMEDIA), lactose monohydrate (LM), magnesium stearate (SM) (Stanchem, Poland). Capsules sealed with DIOX were prepared, in total 5 formulations (F1, F2, F3, F4, F5), with identical active ingredient content, but with different composition of EX. The "Dissolution" test was performed in accordance with the European Pharmacopoeia 11th ed., chapter 2.9.3. "Dissolution test for solid dosage forms" using the ELECTROLAB DISSOLUTION TESTER (Chem Lab Belgium) dissolution apparatus, with 8 positions and vessels with a useful volume of 1000 ml. As dissolution media, 0.1 M hydrochloric acid (pH=1-2) and phosphate buffer solution (pH=6.8) were used (because they present environments with a pH close to gastric and intestinal juice) at a temperature of 37 ± 0.5°C. Stirring element: rotating basket, with a rotation speed of 100 rpm. 10 ml samples were taken manually in the following time sequence: 5, 10, 15, 20, 30, 45 and 60 min. The samples were followed by replacement with degassed blank medium, to maintain the conditions and prevent hydrodynamic changes related to volume decreases. Quantitative analysis was performed spectrophotometrically, λ max = 257 nm, solvent – ethanol (96%). The same procedure was applied for all sample sets, to ensure the comparability of the data obtained for the analyzed formulations. After researching the dissolution profile of DIOX in acidic and basic environments, it was found that the release of the active substance in acidic environments is better. The kinetic parameters of DIOX dissolution from sealed capsules were calculated. Following the analysis of the results, it can be concluded that the most optimal formulation is F5 (D 40%, SM 1%, LM 39%, CMC 20%).

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PP2.6

Evaluation of complexometric titration and atomic absorption spectroscopy in the assay of magnesium aspartate

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Magnesium is an indispensable mineral for the human body, being the fourth most abundant in the body and having a fundamental role in cellular processes. An adult body contains around 25g of magnesium, of which approximately 50% to 60% is found in the bone structure, and the rest is mainly found in soft tissues and plasma where it functions as a cofactor for over 300 essential enzymatic reactions. Due to its importance in biological processes and industrial applications, magnesium is a key element in the formulation of drugs, nutritional supplements, metal alloys and other chemical compounds. Therefore, the development of efficient, rapid and reliable analytical methods for the determination of this element is vital [1]. In recent years, the analytical methods used for the quantitative determination of magnesium have evolved significantly, with increasingly sensitive, selective and rapid techniques being developed. Among the most widely used methods for the analysis of magnesium, complexometric assay and atomic absorption spectroscopy (AAS) stand out due to their efficiency and frequent applicability [2]. The objective of this study was to compare two analytical methods for magnesium aspartate assay: complexometric titration and AAS, with emphasis on reproducibility and reliability. In complexometry, magnesium ions form stable complexes with Na_2EDTA using Eriochrome Black-T as indicator. In parallel, quantitative evaluation was performed by AAS (AAS-1 Carl Zeiss Jena) at the Institute of Chemistry, based on the characteristic absorption wavelength of magnesium at 286 nm. The experimental results demonstrated that the magnesium content in the combined powder was 99.38% (RSD < 2) by complexometric titration and 95.7% (RSD < 2) by AAS. Statistical analysis revealed that for all three series of tested samples, the values obtained for the Fisher test (F_{exp}) were lower than the critical value F_{crit} = 6.39 at the 95% confidence level, confirming the absence of significant differences between the variances. Both methods, therefore, exhibited comparable precision. Furthermore, application of the Student's t-test yielded values of t_{exp} = 3.93, which exceeded the critical threshold at $\alpha = 0.05$ (t_{crit} = 2.31) but remained below the threshold at $\alpha = 0.02$ (t_{crit} = 4.50). These findings indicate the absence of systematic error at the confidence level $\alpha = 0.002$, thereby validating the reliability of both methods. In conclusion, the comparative evaluation demonstrates that complexometric titration and atomic absorption spectroscopy are both suitable for the quantitative assay of magnesium aspartate, each presenting specific advantages. Complexometric titration remains a simple, rapid, and cost-effective technique widely applicable in routine laboratory settings, while AAS provides higher sensitivity and specificity, particularly valuable when analyzing complex matrices.

Keywords: magnesium aspartate, complexometric titration, atomic absorption spectroscopy, pharmaceutical analysis, assay validation.

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References

1. Waminathan R. Metabolismul magneziului și tulburările sale, Clinical Biochemistry, 1988, 21(4), 297-308. https://doi.org/10.1016/0011-5029(88)90013-2.
2. Malon, A., Maj-Zurawska M. The new methods of determination of Mg^{2+}, Ca^{2+}, Na^{+} and K^{+} ions in erythrocytes by ion selective electrodes. Sensor and Actuators B: Chemical, 2005, 108, 828-831. https://doi.org/10.1016/j.snb.2004.12.091

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PP2.7

Characteristic features of diabetes in NMR spectra

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Introduction. Nuclear magnetic resonance (NMR) based lipidomics provides an advanced approach for detailed characterization of lipoproteins, beyond the capabilities of conventional lipid profiling. In diabetes, where dyslipidemia is a key determinant of cardiovascular risk, NMR lipidomics may reveal specific metabolic signatures relevant to disease progression and the development of complications. The aim of the study was to characterize the lipid profile in individuals with diabetes using NMR spectroscopy, including standard parameters and the added value of extended lipidomic measures.

Material and methods. The pilot study included 12 individuals with type 1 diabetes. Biological samples were collected and analyzed at the "Petru Poni" Institute of Macromolecular Chemistry, Iași, Romania. The samples were subjected to NMR-based lipidomic analyses. Statistical analysis was performed using SPSS, and the data are presented as mean±standard deviation (M±SD).

Results.The study included 12 individuals with type 1 diabetes (41,7% men, 58,3% women; mean age 40,9±10,3 years). Conventional biochemical analysis revealed a mean total cholesterol of 6,04±1,23 mmol/L, LDL cholesterol 3,36±0,94 mmol/L, HDL cholesterol 1,47±0,28 mmol/L, and triglycerides 1,52±0,73 mmol/L. NMR-based lipidomics provided extended characterization, revealing apoA1 levels of 149,45±18,85 mg/dL, apoA2 of 28,92±3,96 mg/dL, and apoB100 of 101,31±33,84 mg/dL. In addition, NMR quantified advanced particle-based metrics, with a mean LDL particle number of 1518,33±441,89 nmol/L and a total apoB100 particle number of 1896,25±512,9 nmol/L.

Discussions. The present study highlights the added value of NMR-based lipidomics in characterizing the lipid profile of individuals with type 1 diabetes. Conventional biochemical analysis confirmed a dyslipidemic pattern typical of diabetes, with elevated total and LDL cholesterol, reduced HDL cholesterol, and moderate hypertriglyceridemia. In contrast, NMR spectroscopy provided an extended view of lipoprotein structure and composition. The quantification of apolipoproteins showed moderately reduced ApoA1, suggestive of impaired HDL functionality, and elevated ApoB100, consistent with an atherogenic phenotype. NMR revealed increased LDL and apoB100 particle counts, parameters not captured by routine lipid testing. These measures may be more strongly associated with cardiovascular risk than cholesterol content, as smaller, cholesterol-depleted LDL particles may exert disproportionate atherogenic effects. Nevertheless, given the exploratory design and small sample size of this study, these exploratory findings need validation in larger cohorts to clarify the added prognostic value of NMR lipidomics in diabetes.

Conclusion. NMR-based lipidomics allowed a detailed characterization of lipid profiles in individuals with diabetes. The results indicate that extended lipidomic parameters may serve as complementary biomarkers for cardiovascular risk assessment and metabolic profiling.

Key words: diabetes, dyslipidemia, lipidomics, NMR

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PP2.8

Preliminary results from the PoliGeNReg Project: a bicentric cross-border inventory of ADPKD cases in Romania and the Republic of Moldova

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Background. Autosomal Dominant Polycystic Kidney Disease (ADPKD) is a genetically determined disorder and ranks as the 4th leading cause of renal replacement therapy worldwide. Despite a reported prevalence of 1/1,000 in population-based studies and 2–4/10,000 in healthcare database analyses, the true burden of ADPKD remains uncertain [1].

Material and methods. The PoliGeNReg project is a two-year cross-border initiative aimed to establish a comprehensive registry of ADPKD patients in North-Eastern Romania and the Republic of Moldova. The registry integrates clinical, epidemiological, and genetic data to improve disease understanding, monitoring, and individualized care.

Results. A retrospective analysis was conducted using standardized data from existing databases of nephrology centers in Iași and Chișinău. A total of 522 patients were identified: 57.87% from Romania and 42.13% from Moldova. Most patients (over 55%) were aged over 55 years, suggesting an aging cohort and possible delays in diagnosis. Less than 10% of patients were under 40 in both regions. The sex ratio was balanced, with a slight female predominance (54.5%) in Chișinău. A heatmap analysis of comorbidities revealed clear age-related trends. Individuals under 40 had minimal comorbidities, while patients over 55 exhibited high rates of hypertension, cardiovascular disease, anemia, diabetes, and dyslipidemia. The distribution of CKD stages differed between regions: in Chișinău, all CKD stages (G1–G5) were represented, with G3 being most prevalent, and G5 (end-stage kidney disease) most dominant in Iași.

Conclusions. These findings highlight the clinical heterogeneity of ADPKD and the need for early diagnosis, standardized monitoring, and tailored interventions. The next steps of the project will focus on genetic testing, refined staging, and improved long-term follow-up to enable personalized treatment strategies and better prognostic stratification.

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References

1. Kidney Disease: Improving Global Outcomes (KDIGO) ADPKD Guidelines, 2025.

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PP2.9

The role of salivary interleukins in the prediction of caries risk in children

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Introduction. Dental caries (DC) in children remains a significant public health concern both globally and within our national population. The complex nature and multifactorial etiology of the disease highlight the need for personalized management strategies. Early identification of caries risk is a priority in pediatric dentistry due to the potential complications arising from the progression of the disease. Recent advancements in artificial intelligence and machine learning technologies have enabled the development of increasingly accurate predictive models, capable of identifying complex interactions among various risk factors. These innovations offer promising tools for improving early diagnosis, risk assessment, and the implementation of targeted preventive measures.

Aim of the study is to assess the concentration of pro-inflammatory and anti-inflammatory cytokines in oral fluid (OF) and to investigate their potential impact on the susceptibility of children to DC.

Materials and methods. A prospective observational cohort study was carried out involving 398 children. Participants were divided into two groups: the study group (Gr_1), comprising 132 children diagnosed with DC, and the control group (Gr_0), including 266 caries-free children. The evaluation included caries experience indices, oral hygiene status, and the analysis of biomarkers in OF. Caries risk assessment was performed using the *Cariogram software* and by evaluating the salivary count of *Streptococcus mutans* with the *Saliva-Check Mutans kit.* To identify predictive factors for the development of DC, a multivariable linear regression model (linearMod) was constructed. The study was conducted in accordance with ethical requirements.

Results. The mean caries experience was 4.74 ± 2.65 (95% CI: 4.3–5.2, $p < 0.001$) for the DMFT/dmft ± SD index and 8.06 ± 4.9 (95% CI: 7.2–8.9, $p < 0.001$) for the DMFS/dmfs ± SD index. A high salivary *Streptococcus mutans* count, >5 × 10^5 CFU/mL, was observed in 53.0% ($p < 0.001$) of children in the study group (Gr_1) and 8.6% of subjects in the control group (Gr_0), indicating an increased risk of developing carious lesions in the future. Conversely, a low SM count in oral fluid, <5 × 10^5 CFU/mL, associated with low caries risk, was found in 47.0% ($p < 0.001$) of children affected by dental caries and 91.4% of caries-free subjects. Levels of pro-inflammatory interleukins (IL-1, IL-6, IL-12) and the anti-inflammatory interleukin (IL-10) were evaluated. IL-1 levels were elevated in children affected by dental caries and lower in caries-free children. Differences in IL-6, IL-12, and IL-10 levels in oral fluid between Gr_1 and Gr_0 were not statistically significant.

Conclusions. IL-1 is a pro-inflammatory interleukin with significant predictive value for assessing caries risk in children. The integration of salivary biomarkers into complex predictive models may enhance early identification of children at high risk for dental caries and support personalized preventive strategies in pediatric dentistry.

Keywords: dental caries, children, pro-inflammatory cytokines, anti-inflammatory cytokines, prevention.

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PP2.10

Mother-child salivary *Streptococcus mutans* levels: a key marker for early diagnosis of severe early childhood caries

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Introduction. Severe early childhood caries(S-ECC) represents a major public health issue, with consequences for child development and a complex etiology in which *Streptococcus mutans* plays a central role. The identification of reliable clinical and prognostic markers is essential for early diagnosis and prevention of S-ECC.

Materials and methods. The study included 60 mother-child pairs, divided into two groups: the research group Gr1 consisted of 30 pairs with children diagnosed with S-ECC and the control group Gr0 consisted of 30 pairs with healthy children. The following indices of carious experience were evaluated: dmft/dmfs indices for children, DMFT/DMFS indices for mothers, oral hygiene index(OHI), as well as salivary levels of *Streptococcus mutans* using the *Saliva-Chek Mutans Kit(GC)*.

Results. Children with S-ECC presented a significantly higher dmft scores (4.2±2.5) and dmfs scores (9.3±5.0) compared with control group, $p<0.001$. Mother of children from research group Gr_1 had a higher caries experience (DMFT=7.0±3.0; DMFS=11.8±7.2), than those in Gr0 ($p\leq0.002$). The OHI indices was significantly higher in children with S-ECC (1.90±0.60 vs. Gr_0 0.90 ± 0.30; $p<0.001$). Increased level of *Streptococcus mutans* were detected in 73.3% of children with S-EEC and 66.7% at their mothers, significantly more frequent than in controls group ($p<0.01$).

Conclusions. Salivary levels of *Streptococcus mutans* proved to be reliable clinical and prognostic marker of severe early childhood caries. Children affected by S-ECC and their mothers demonstrated increased caries experience and deficient oral hygiene, highlighting both bacterial transmission and the impact of suboptimal hygiene behaviors. Salivary *Streptococcus mutans* levels confirm their role as a clinical and prognostic marker of S-ECC. The results of the study highlight the importance of implementation of family-centered preventive strategies and incorporating of salivary biomarker evaluation in assessing caries risk in young children.

Keywords: dental caries, children, early childhood, Streptococcus mutans, cariogenic risk.

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PP2.11

Natural biomaterials-based formulations: aspects regarding their biocompatibility

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Natural biomaterials play a critical role in tissue engineering due to their close resemblance to the native extracellular matrix (ECM), which is essential for supporting cellular behavior and promoting tissue regeneration. Their biological origin often allows them to contain intrinsic bioactive molecules that facilitate cell adhesion, proliferation, differentiation, and migration—key processes in tissue repair and development [1]. The importance of these materials also lies in their ability to integrate naturally with host tissue, reducing the risk of immune rejection and enhancing long-term functionality. In addition to their biological relevance, natural biomaterials offer several practical advantages. They are typically biocompatible, minimizing inflammatory responses, and biodegradable, enabling the scaffold to be gradually replaced by newly formed tissue without requiring surgical removal. Many natural materials also have low toxicity, with degradation byproducts that are non-harmful to surrounding tissues. Furthermore, their inherent bioactivity and ease of chemical modification allow for the design of scaffolds tailored to specific tissue environments. Collectively, these attributes make natural biomaterials indispensable in the design of safe, effective, and functional tissue engineering systems [2].

Bioadhesion is a critical property for biomaterials because it enables stable and functional interaction between the material and biological tissues or cells, which is essential for successful integration and therapeutic outcomes. Bioadhesive surfaces enhance cell attachment, spreading, and proliferation, providing a favorable environment for tissue regeneration. Without sufficient adhesion, cells may detach or fail to survive, limiting the effectiveness of the scaffold or implant. Strong bioadhesion improves tissue integration, allowing the biomaterial to bond with surrounding tissues rather than being encapsulated or rejected, which enhances healing and long-term performance. In dynamic or fluid-filled biological environments, such as the gastrointestinal tract or vascular system, bioadhesion also contributes to positional stability, preventing the displacement of scaffolds, wound dressings, or drug delivery systems and ensuring they remain in place for optimal function. Additionally, the adhesive interface between cells and biomaterials plays a role in cellular signaling, triggering intracellular pathways that regulate processes such as cell differentiation, migration, and survival—key factors in tissue engineering and regenerative medicine. Finally, biomaterials with good bioadhesive properties are less likely to induce a foreign body response, as the strong and biocompatible interface reduces inflammation and fibrous encapsulation, increasing the likelihood of long-term biocompatibility and implant success [3].

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References

1. Ratner, B. D., Hoffman, A. S., Schoen, F. J., & Lemons, J. E. (Eds.). (2012). Biomaterials Science: An Introduction to Materials in Medicine (3rd ed.). Elsevier.
2. Filip, D., Macocinschi, D., Zaltariov, M.-F., Gafitanu, C. A., Tuchilus, C. G., Bele, A., Ciubotaru, B.-I., Stoleru, E., & Bargan, A. (2022). Mucoadhesive and Antimicrobial Allantoin/β Cyclodextrins-Loaded Carbopol Gels as Scaffolds for Regenerative Medicine.*Gels*,*8*(7), 416. https://doi.org/10.3390/gels8070416
3. Place, E. S., Evans, N. D., & Stevens, M. M. (2009). Complexity in biomaterials for tissue engineering. *Nature Materials*, 8(6), 457–470. https://doi.org/10.1038/nmat2441

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PP2.12

A new generation of antimicrobial agents based on multicomponent systems

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Multicomponent systems based on biopolymers and inorganic nanaoparticles (NPs) have been designed as a new class of non-cytotoxic and bioactive materials of interest in applications as antimicrobial films and drug delivery systems, scaffolds in regenerative medicine, wound dressing, etc. [1-2]. The advantages of these materials arise from the synergy of different natural constituents that can be combined in different ratios to consolidate and improve mechanical and chemical resistance and to increase the biocompatibility. The intermolecular crosslinks created between the components can also ensure self-healing ability, adhesion of cells, gradual degradation in physiological media, and adequate hydrophilic-hydrophobic balance. ZnO, AgNPs, nano-SiO_2, CeO have already demonstrated antimicrobial activity, higher stability, UV absorption or barrier properties [3,4].

In this study we report multicomponent composites based on chitosan, starch, gelatin and inorganic NPs (ZnO and Fe_3O_4) as antimicrobial agents for biomedical applications. The amino functionality of chitosan can easily interact with gelatin, starch also can be included by intermolecular interactions ensuring low hemolysis risk and wound sealing for long-term effectiveness. The addition of NPs favored better the connectivity between all the components and increased the hydrophily of the multicomponent blends. It was found that antimicrobial activity on several species of bacteria (*Bacillus sp*. and *Pseudomonas sp*.) and fungi (*Penicillium frequentas, Fusarium, Aspergillus fumigatus*) was dependent on the ratio between the blend components and the added NPs.

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References

1. J. Matmin, N.A.N.N. Malek, N.S. Sani, Biodegradable inorganic nanocomposites, in: G.A.M. Ali, A.S.H. Makhlouf (Eds.), Handbook of Biodegradable Materials, Springer, Cham, 2022, pp. 1–40, https://doi.org/10.1007/978-3-030-83783-9_23- 1.
2. S.A. Mathew, S. Arumainathan, Crosslinked chitosan-gelatin biocompatible nanocomposite as a neuro drug carrier, ACS Omega 7 (2022) 18732–18744.
3. P. Widiyanti, R. Prastyani, Collagen-chitosan-glycerol-HPMC composite as cornea artificial candidate, J. Biomim. Biomater. Biomed. Eng. 42 (2019) 14–21.
4. Y. Zare, I. Shabani, Polymer/metal nanocomposites for biomedical applications, Mater. Sci. Eng. C 60 (2016) 195–203.
5. D. Filip, D. Macocinschi, S. L. Nica, M. Asandulesa, B. Condurache, E. Stoleru, D. M. Rata, A. Bargan, M.-F. Zaltariov, Hybrid green bionanocomposites based on chitosan/starch/gelatin and metallic nanoparticles for biological applications, Int. J. Biol. Macromol. 253 (2023) 127571.

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PP2.13

"OncoSensLip" - optimization of process and formulation variables in the design of pH-sensitive liposomes for anticancer drug delivery

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Introduction. One of the pre-requisites for eradication of the cancerous cells is to attain sufficient cytoplasmic levels of the antineoplastic drugs. The acidic pH of the tumor endosomes can be utilized to enhance intracellular levels of the drugs. Recently, the role of pH-sensitivity in liposomes has been investigated for enhancing the cellular delivery and pharmacokinetic properties.

Aim and objectives. The aim and objectives of the proposed project "OncoSensLip" lies in several key areas of exploration: the relationship between formulation, process variables, pH-sensitivity and the potential for broader applicability in oncological areas, where local pH changes play a role.

Results. To accomplish the project "OncoSensLip" objectives, several activities that will merge in a robust experimental plan will be carried out. Therefore, optimization of lipid composition of pH-sensitive liposomes using different phospholipids, investigation of the effects of preparation methods (thin-film hydration with extrusion/sonication and microfluidics), evaluation of properties, such as size, stability, encapsulation efficiency, loading capacity, pH-triggered release and in vitro biological actions, assessment of the biological effects on normal and tumour cell lines are all aimed at providing valuable insights into the preparation of liposomes, with a high potential for scalable transfer on the path of product development.

Conclusions. The development of different types of liposomal formulation drugs will address a need for innovation in the therapy of cancer, being well related to the aim of the currently running Horizon 2020 ERA-Chair project at IRO Iași, under which the *OncoSensLip* project was awarded. Equally important, the project will allow us to explore the 'know-how' for both teams in line with their background in order to reach the optimum of the knowledge transfer and create a team capable of securing additional funds.

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PP2.14

Erythrocyte glucose-6-phosphate dehydrogenase activity in bronchial asthma: effects of sulfated polysaccharides

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Introduction. Excess of reactive oxygen species (ROS) and reactive nitrogen species (RNS) contribute to chronic airway inflammation in bronchial asthma (BA). Antioxidant supplementation may help restore the oxidant/antioxidant balance. Polysaccharides have been reported to modulate airway inflammation [3]. Polysaccharides derived from various algae exhibit free radical scavenging activity both in vivo and in vitro [2]. In Moldova, original biotechnological models for the controlled cultivation of *Spirulina platensis* have been developed, enabling the extraction and purification of sulfated polysaccharides (SPS) [4]. Since the immunobiochemical mechanisms of cyanobacterial SPS in respiratory disorders remain insufficiently clarified, this research provides a promising avenue for the development of effective and safe therapeutic agents for asthma management.

Materials and methods. In vitro experiments were performed using biological material collected from patients with BA. Study design included: control group, patients with mild persistent BA, moderate persistent BA, and severe persistent BA. SPS were tested at concentrations of 50 and 100 μg/ml. G6PD activity was assessed in erythrocyte lysates. The determination method is based on the ability of the enzyme to catalyze the oxidation of glucose-6-phosphate to 6-phosphogluconolactone in the presence of NADP, which is subsequently reduced to $NADPH_2$ [1]. Statistical analysis was performed using *StatsDirect* and *Statistica 6.0* software.

Results. A significant increase ($p < 0.01$) in G6PD activity was observed in conditionally healthy individuals exposed to SPS at both tested concentrations. In mild persistent BA, G6PD activity remained at the lower boundary of baseline values; however, compared to the control group, a significant elevation ($p < 0.001$) was noted with both SPS doses. In moderate persistent BA, G6PD activity exceeded control values by approximately three-fold ($p < 0.001$) across all groups, though it was reduced by 27% (SPS 50 μg/ml) and 31% (SPS 100 μg/ml) compared with baseline values. In severe persistent BA, SPS treatment induced a significant activation of G6PD compared with both the control group ($p < 0.001$) and initial values ($p < 0.01$).

Conclusions. The SPS-induced increase in G6PD activity suggests an enhancement of the cellular NADPH pool. Taking in account that glucose-6-phosphate dehydrogenase (G6PD) plays a key role in generating NADPH, which is essential for the synthesis of reduced glutathione, a major cellular protector against oxidative injury, SPS can contribute to the maintenance of a high reducing potential and for attenuation of the airway inflammation in patients with BA.

References

1. Gudumac V., Tagadiuc O., Rîvneac V., Sardari V., Pantea V., Andronache L., Ştîrba O. Biochemical Investigations: Methodological Development. Vol. II. Micromethods. Nicolae Testemițanu State University of Medicine and Pharmacy. Chişinău: Elena V.I. Printing House, 2010. 97 p. ISBN 978-9975.
2. Jiao G., Yu G., Zhang J., Ewart H. S. Chemical structures and bioactivities of sulfated polysaccharides from marine algae. In: Mar Drugs. 2011, 9:196–223.
3. Lin R., Liu X., Meng Y., Xu M., Guo J. Effects of Laminaria japonica polysaccharides on airway inflammation of lungs in an asthma mouse model. In: Multidiscip. Respir. Med. 2015, 10(1):20.
4. Rudic V. Phycobiotechnology – fundamental research and practical achievements. In: Elena-VI Publishing House, Chisinau, 2007, 364 p.

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PP2.15

The impact of diabetes mellitus on pulmonary tuberculosis through the lens of inflammation marker exegesis

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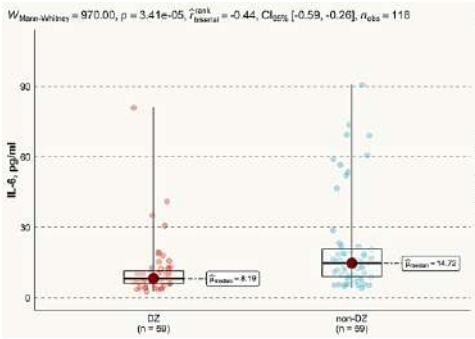
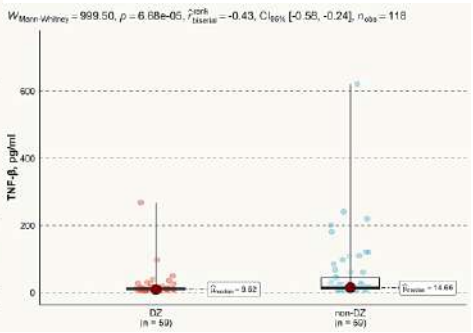
Introduction. The double burden of tuberculosis (TB) and diabetes mellitus (DM) represents a major public health challenge that demands urgent and integrated approaches. According to 2024 World Health Organization data, a total of 8.2 million people were newly diagnosed with TB in only one year. Diabetes mellitus has also increased rapidly worldwide. Regionally, in Europe a prevalence of 17.31%. of patients with DM and TB has been observed.

Materials and methods. The prospective study was carried out within "Chiril Draganiuc" Pneumology Institute. The study was approved by the Research Ethics Committee of the "Nicolae Testemițanu" State University of Medicine and Pharmacy (decision no. 31 of 18.05.2019). The study included 118 patients, divided into two subgroups: group L_1, consisting of 59 patients with pulmonary tuberculosis and diabetes mellitus, and group L_2, consisting of 59 patients with pulmonary tuberculosis without diabetes mellitus. Serum levels of IL-6 and TNF-β were measured by Enzyme-Linked Immunosorbent Assay (ELISA). All participants were evaluated both before and after hospital treatment.

Results. The results indicate that, prior to treatment, patients in group L_2 exhibited significantly higher serum levels of IL-6 (21.9 vs. 16.1 pg/ml, $p<0.002$) and TNF-β (58.4 vs. 39.5 pg/ml, $p<0.016$) compared to those in group L_1 (figure 1). Following treatment, the levels of both markers decreased in both groups, although higher values persisted in patients from group L_2 compared to group L_1. Specifically, post-treatment concentrations were 21.4 vs. 11.2 pg/ml ($p<0.001$) for IL-6 and 50.6 vs. 18.6 pg/ml ($p<0.001$) for TNF-β (figure 2).



(Figure 1). Median serum IL-6 level in groups



(Figure 2). Median serum TNF-β level in groups

Conclusion. These findings suggest that patients with pulmonary tuberculosis without diabetes (group L_2) exhibit a more pronounced inflammatory response, as reflected by higher IL-6 and TNF-β levels, both before and after treatment. Although therapy reduced cytokine concentrations in both groups, residual elevations in group L_2 indicate a sustained pro-inflammatory state.

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PP2.16

The potential use of spirulina derived substances in periodontal tissue regeneration

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Spirulina (*Arthrospira*) is a filamentous cyanobacterium that has been recognized as a nutrient-dense functional food rich in proteins (superfood), essential fatty acids, vitamins, and bioactive compounds such as phycocyanin. Spirulina was evaluated also for antioxidant, anti-inflammatory, immunomodulatory, and antimicrobial activities, leading to growing interest in its potential applications in oral health [1-3].

Our aim was to synthesise existent evidence on the potential uses of spirulina in the management of periodontal disease, along with our own experience regarding the employment of this bioactive substance in various dental conditions.

Animal models help simulate host–pathogen interactions, drug pathways, and tissue regeneration. Rodent studies show spirulina may reduce alveolar bone loss, lower pro-inflammatory cytokines (TNF-α, IL-1β, IL-6), and influence oral tumor development, albeit anatomical and immune differences limit their comparability to humans [2,4].

Porcine models are valued in dental and oral research because of their anatomical, histological, and physiological similarities to human oral tissues [4]. In our previous studies, the potential of spirulina in bone regeneration was assessed in a pig model, where mandibular bone defects were treated with Bio-Oss alone or combined with a spirulina-derived bioactive substance (BioR® formulation). After 5 months, bone density values did not differ significantly from controls (1600 ± 44.7 HU, 1695 ± 47.6 HU, 1720 ± 50.8 HU; $p = 0.085–0.722$). BioR® supported osteoconduction and osteoinduction without pathological bone resorption, antigenic reactions remained mild [5].

In a clinical study conducted by our team, BioR® significantly improved outcomes in chronic catarrhal gingivitis and periodontitis: the deodorant effect was 3.9 times greater in mild vs. moderate gingivitis ($p = 0.048$), edema resolved faster after 3 days ($p = 0.00012$), and disappeared in all patients by day 7. Intragingival use was effective, while intramuscular administration offered broader action with fewer side effects, enhancing therapy especially in severe periodontal disease [5].

Evidence from animal models and clinical trials suggests that spirulina may support periodontal health by reducing inflammation, limiting alveolar bone loss, and modulating host responses. While these findings are promising, further clinical studies are needed to confirm its potential as an adjunct in dental practice.

References

1. G. Andrade, T. F. Labarca, V. Llanca, at al. "Using Spirulina as an adjuvant to the treatment of Periodontitis: a systematic review of clinical trials," Feb. 09, 2023, In Review. doi: 10.21203/rs.3.rs-2539298/v1.
2. M. S. Kang, J.-H. Moon, S. C. Park, et al. "Spirulina maxima reduces inflammation and alveolar bone loss in Porphyromonas gingivalis-induced periodontitis," Phytomedicine, vol. 81, p. 153420, Jan. 2021, doi: 10.1016/j.phymed.2020.153420.
3. V. R. K. Kaipa et al., "Antioxidant effect of spirulina in chronic periodontitis," Medicine, vol. 101, no. 50, p. e31521, Dec. 2022, doi: 10.1097/MD.0000000000031521.
4. H. S. Oz and D. A. Puleo, "Animal Models for Periodontal Disease," BioMed Research International, vol. 2011, no. 1, p. 754857, Jan. 2011, doi: 10.1155/2011/754857.
5. V. Fala, BioR - Baza optimizării proceselor de regenerare tisulară. Universitatea de Stat de Medicină și Farmacie „Nicolae Testemițanu", 2014.

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PP2.17

The potential application of the rapid aMMP-8 test in population-based periodontal screening

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Periodontal disease is among the most prevalent chronic conditions worldwide, with significant implications for both oral and systemic health, as well as for quality of life [1,5]. Early detection remains challenging due to the asymptomatic nature of initial stages and the limitations of conventional diagnostic methods, which primarily reflect past tissue destruction rather than current disease activity [4]. In recent years, salivary biomarkers have emerged as promising non-invasive diagnostic tools, with activated matrix metalloproteinase-8 (aMMP-8) established as a validated indicator of periodontal tissue degradation and active inflammation. [1,2].

The rapid aMMP-8 test, based on lateral-flow technology, provides results within approximately five minutes and has demonstrated sensitivities ranging from 75–96% and specificities above 80% in meta-analyses and multicenter trials [2,3]. These diagnostic performances support its use as a population-level screening tool, offering clear advantages over traditional methods: higher accuracy, speed, cost-effectiveness, and greater patient acceptability.

In our experience, the initial testing conducted by us shows beneficial results for using this technology as a general screening kit, especially effective for feasible and fast deployment in larger populations.

By enabling the early identification of high-risk individuals, the test facilitates timely preventive and therapeutic interventions, thereby reducing the burden of periodontal disease on public health systems [1].

Its integration into community screening programs could represent a paradigm shift in periodontal diagnostics, contributing to the development of a new interdisciplinary field—oral clinical chemistry. Although economic and logistical challenges persist, advances in standardization, digital health infrastructure, and artificial intelligence may support the feasibility of large-scale implementation [4]. Future research directions should include combining aMMP-8 with other salivary biomarkers and predictive algorithms to achieve increasingly personalized and effective prevention and treatment strategies [5].

References

1. Sorsa T, Gieselmann DR, Arweiler NB, Hernández M. A quantitative point-of-care test for periodontal and dental peri-implant diseases. Nat Rev Dis Primers. 2017;3:17069.
2. Rathnayake N, Gieselmann DR, Heikkinen AM, Tervahartiala T, Sorsa T. Salivary diagnostics for oral diseases: A potential tool for clinical decision-making. J Clin Periodontol. 2015;42(9):799–807.
3. Heikkinen AM, Nwhator SO, Rathnayake N, Mäntylä P, Vatanen P, Sorsa T. Pilot study on oral health status as assessed by an active matrix metalloproteinase-8 chairside test in adolescents. J Periodontol. 2016;87(1):36–42.
4. Sanz M, Herrera D, Kebschull M, Chapple I, Jepsen S, Tonetti MS. Treatment of stage I–III periodontitis—The EFP S3 level clinical practice guideline. J Clin Periodontol. 2020;47(S22):4–60.
5. World Health Organization (WHO). Global oral health status report: Towards universal health coverage for oral health by 2030. Geneva: WHO; 2022.

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PP2.18

Caries risk assessment using the saliva check mutans microbiological test

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Dental caries is one of the most common chronic diseases, with a significant impact on oral and general health. Its etiopathogenesis is complex, involving microbial, dietary, environmental and individual factors [1]. Among bacterial agents, *Streptococcus mutans* is considered the main microorganism involved in the initiation of carious lesions, due to its ability to produce acids by fermenting carbohydrates and to adhere to the tooth surface. The assessment of the level of *S. mutans* in saliva can provide essential information for the early detection of caries risk [2].

The aim of this study is to highlight the importance of using the Saliva-Check Mutans test as a simple, microbiological, rapid and non-invasive method to identify the level of *S. mutans* in saliva, thus contributing to the assessment of the risk of dental caries.

The Saliva-Check Mutans test uses an unstimulated saliva sample collected from the patient. The sample is applied to strips with specific *S. mutans* antibodies. The development of bacterial colonies is compared with a reference scale, the results being classified into three levels: low ($<10^5$ CFU/ml), moderate (10^5–10^6 CFU/ml) and high ($>10^6$ CFU/ml). Analysis of the samples showed a direct correlation between the concentration of *S. mutans* in saliva and the prevalence of caries [5]. Patients with high values ($>10^6$ CFU/ml) presented an increased number of caries, compared to those with low levels, in which the caries incidence was reduced. Previously, it was also observed that patients with poor oral hygiene and frequent carbohydrate consumption recorded higher bacterial values [5]. The Saliva-Check Mutans test represents a valuable tool for the assessment of caries risk, due to its rapid, simple and non-invasive nature. The results obtained highlight the fact that an increased level of *Streptococcus mutans* in saliva is associated with a higher incidence of dental caries. The use of this test in dental practice allows early identification of high-risk patients and implementation of personalized preventive measures. However, the assessment must be complemented with other risk factors: oral hygiene, diet, salivary flow, for a complex and accurate diagnosis [3].

References

1. Wennerholm K, Emilson CG. *Comparison of Saliva-Check Mutans and Saliva-Check IgA Mutans with the Cariogram for caries risk assessment.* European Journal of Oral Sciences. 2013;121(5):389-393.
2. Gao XL, Seneviratne CJ, Lo EC, Chu CH, Samaranayake LP. *Novel and conventional assays in determining abundance of Streptococcus mutans in saliva.* International Journal of Paediatric Dentistry. 2012;22(5):363-368.
3. Kaur R, Jain S, Kaur H. *Evaluation of salivary mutans streptococci levels and caries experience in children: A comparative study.* J Indian Soc Pedod Prev Dent. 2019;37(3):254-258.
4. Streptococcus Mutans and its Influence on Dental Status. *Česká Stomatologie a Praktické Zubní Lékařství.* 2016.
5. Kaur R, Jain S, Kaur H. *Evaluation of salivary mutans streptococci levels and caries experience in children: A comparative study.* J Indian Soc Pedod Prev Dent. 2019;37(3):254-258.

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PP2.19

Aseptic prostatitis – histopathological identification of the optimal experimental model

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Introduction. Chronic non-bacterial prostatitis (CP/CPPS) is a frequent condition with unclear pathogenesis and limited therapeutic options. Several inflammatory rodent models, including carrageenan-induced, ethanol-induced, and autoimmune prostatitis, are used to reproduce histological features of the disease and test novel therapies [1,2]. Comparative studies emphasize that the severity and reproducibility of tissue damage are critical for selecting an optimal preclinical model [3,4].

Aim. To identify the most relevant histopathologic model of aseptic prostatitis for preclinical use.

Methods. Wistar rats (3 months) received intraprostatic carrageenan 1% or 3%, ethanol 50%, Freund's adjuvant, or urethral ligation. Prostates were collected at 14 and 28 days, stained (H&E), and microscopically evaluated.

Results. Carrageenan 1%, ethanol, and ligation produced minimal lesions. Carrageenan 3% caused moderate inflammation at both time points, while Freund's adjuvant induced severe lymphoplasmocytic and necrotic changes with disrupted acinar structure.

Conclusions. Carrageenan 3% reproducibly induces characteristic, moderate histopathologic changes, making it suitable as a balanced preclinical model of aseptic prostatitis.

Keywords: aseptic prostatitis, carrageenan, histopathology, experimental models.

References

1. H. He, J. Wang, L. Zhang, Preclinical models and evaluation criteria of prostatitis: a comparative review, Front. Immunol. 14 (2023) 1183895. https://doi.org/10.3389/fimmu.2023.1183895
2. X. Li, Z. Wang, J. Chen, Identification of proteomic markers in chronic prostatitis using the experimental autoimmune prostatitis mouse model, Int. J. Mol. Sci. 26 (2025) 4562. https://doi.org/10.3390/ijms26094562
3. O. Aydogdu, M. Malde, D. Wilcock, Induction of chronic prostatitis does not alter innate bladder function but shows cross-organ sensitization, Sci. Rep. 15 (2025) 12987. https://doi.org/10.1038/s41598-025-12987-4
4. S. Song, Y. Liu, T. Zhang, Animal models of chronic prostatitis: lessons and perspectives for translational research, Ther. Adv. Urol. 17 (2025) 17562872251234567. https://doi.org/10.1177/17562872251234567

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PP2.20

A strategic framework for a bi-national ADPKD electronic registry for Romania and the Republic of Moldova: an open-source, interoperable approach for European integration

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Background. Autosomal Dominant Polycystic Kidney Disease (ADPKD) poses a significant healthcare burden in Romania and the Republic of Moldova. However, the lack of a centralized patient registry and the severe fragmentation of clinical data across distinct, non-communicating systems create a critical "data deficit". This deficit impedes epidemiological research, sub-optimizes patient care, and systematically excludes the region's patient population from participation in international clinical trials, thereby limiting access to innovative therapies and creating a structural health inequity.

Methods. This study proposes a strategic framework for the development and implementation of a bi-national electronic registry for ADPKD. The framework is founded on a "Privacy and Security by Design" approach, recommending a federated architecture that respects national data sovereignty while enabling collaborative analysis under strict GDPR compliance. A comparative analysis of open-source software platforms was conducted, evaluating them based on a Total Cost of Ownership model. The framework's single most critical recommendation is the early and mandatory adoption of the Observational Medical Outcomes Partnership (OMOP) Common Data Model (CDM) to ensure the registry is "born interoperable". A robust bi-national governance structure, centered on a Joint Steering Committee and a comprehensive Data Sharing and Use Agreement (DSUA), is also detailed.

Results. The proposed framework provides a comprehensive technical, legal, and operational blueprint for the registry. The federated architecture is identified as the optimal solution for cross-border data collaboration, balancing data security with research needs. The analysis recommends an i2b2/tranSMART platform, leveraged by the OMOP CDM, as the core technical solution to create a standardized and scalable data asset. The governance model ensures equitable partnership, stakeholder inclusion (including patient advocates), and clear rules for data access and use. The primary outcome of implementing this framework will be the creation of a large, well-characterized, research-ready patient cohort, transforming the region into an attractive partner for international research consortia and pharmaceutical trials.

Conclusions. The creation of this bi-national, open-source, and interoperable ADPKD registry is a transformative opportunity to advance patient care and catalyze high-impact research. By aligning with European data standards from its inception, the registry will bridge the existing data deficit, provide access to novel therapies for patients, and build lasting regional research capacity. This initiative will position the Romania-Moldova collaboration not as a passive data contributor, but as a key strategic partner in the continental effort to combat rare diseases, with a clear roadmap for phased integration with the European Reference Network for Rare Kidney Diseases.

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PP2.21

Patterns of biochemical disturbances in patients with suspected mitochondrial disease

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Background. Mitochondrial diseases are a major cause of inherited metabolic dysfunction, exhibiting wide biochemical variability and clinical overlap with other genetic disorders. This study aimed to evaluate biochemical profiles in patients with suspected mitochondrial disease and identify patterns associated with confirmed genetic diagnoses.

Materials and methods. A total of 240 patients with a Nijmegen Mitochondrial Disease Score ≥3 underwent clinical, biochemical, and genetic evaluation. Biochemical analyses included serum lactate, creatine kinase (CK), lactate dehydrogenase (LDH), transaminases (ALT and AST), plasma amino acids, acylcarnitines, ammonia, and urinary organic acids. Genetic testing identified 37 patients with mitochondrial involvement, 44 with non-mitochondrial disorders, and 159 undiagnosed.

Results. Elevated lactate levels were significantly associated with mitochondrial dysfunction (median: 2.9 mmol/L, IQR: 1.5-8.4) compared to non-mitochondrial (1.8 mmol/L, IQR: 0.8-4.9) and undiagnosed patients (1.9 mmol/L, IQR: 1.3-2.5) ($p < 0.001$). Elevated plasma alanine levels were significantly more frequent in the mitochondrial group (32.4%) compared to non-mitochondrial patients (9.1%) ($p = 0.011$), representing the most consistent amino acid marker of mitochondrial dysfunction. Mean CK (281 ± 66 U/L), LDH (541 ± 175 U/L), ALT (93 ± 49 U/L), and AST (247 ± 193 U/L) values were higher in the mitochondrial group, though not statistically significant. No consistent group-specific patterns were observed for ammonia, urinary organic acids, or acylcarnitine profiles.

Conclusion. Biochemical disturbances, particularly elevated lactate and alanine, remain robust indicators of mitochondrial dysfunction. While some metabolic alterations overlap with other genetic conditions, integrated biochemical and molecular data enhance diagnostic precision in suspected mitochondrial disease.

Keywords: Mitochondrial diseases; Biochemical markers; Metabolic profiling.

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PP2.22

Diagnosis of Galactosemia by NMR spectroscopy

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Introduction: Galactosemia is a rare autosomal recessive genetic disorder caused by a deficiency of the enzyme galactose-1-phosphate uridyltransferase (GALT).

Aim: To analyze the correlation between phenotypic characteristics and genotypic profiles in patients diagnosed with GALT, while emphasizing the diagnostic contribution of NMR spectroscopy in metabolic evaluation.

Materials and methods: The study included six patients diagnosed with GALT. Metabolic investigations were performed using proton nuclear magnetic resonance (^{1}H-NMR) spectroscopy to quantify galactose and galactitol levels in urine, in collaboration with the "Petru Poni" Institute of Macromolecular Chemistry, Iași, Romania. Blood galactose concentration was also determined. Molecular confirmation was achieved by Sanger sequencing, identifying pathogenic variants in the GALT gene.

Results: The mean age at symptom onset was two weeks. The clinical phenotype included hypoglycemia, vomiting, hepatosplenomegaly, seizures, and psychomotor and growth retardation. NMR spectroscopy provided high sensitivity in detecting and quantifying galactose and galactitol in urine, with galactose levels ranging from *10,255* to *585,000 mmol/molCrn* and galactitol from *686* to *61,423 mmol/molCrn,* confirming metabolic dysfunction. Elevated blood galactose levels (*15.6–80 mg/dL*) and absent urinary glucose were also noted in several cases. The Q188R variant was predominant, either in homozygosity (one case) or in compound heterozygosity with K285N (three cases), E203L (one case), or an unknown variant (one case). The Q188R/K285N genotype was associated with severe metabolic decompensation, recurrent hypoglycemia, seizures, neurodevelopmental delay, and one fatal outcome. Statistical analysis revealed a significant correlation between this genotype and disease severity ($p = 0.048$, Fisher's exact test).

Conclusions: The Q188R mutation, frequent in the Moldovan cohort, in compound heterozygosity with severe alleles (K285N, E203L), is associated with a severe, multisystemic phenotype. NMR spectroscopy proved to be a highly informative, noninvasive diagnostic tool, enabling early detection of abnormal galactose metabolites and facilitating biochemical confirmation of Galactosemia. These findings highlight the complementary role of metabolic and molecular analyses in establishing an accurate diagnosis and predicting disease prognosis.

Keywords: GALT, NMR-spectroscopy, galactitol, galactose.

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PP2.23

Genetic screening in symptomatic patients: distinguishing spinal muscular atrophy from metabolic disorders

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Background. Infants presenting with hypotonia often exhibit diverse and severe clinical manifestations, thereby highlighting the need for rapid and accurate diagnostic assessment. Due to overlapping features among numerous neuromuscular and metabolic disorders, distinguishing spinal muscular atrophy (SMA) from other etiologies remains challenging [1]. The ubiquitously expressed SMN protein, essential for RNA splicing and cellular maintenance, plays a key housekeeping role in SMA pathogenesis, though its mechanisms are not yet fully elucidated [2]. Genetic testing offers a highly reliable and non-invasive diagnostic tool; however, more than 30 neuromuscular and over 50 metabolic disorders can mimic SMA phenotypes, emphasizing the importance of comprehensive genetic screening in symptomatic patients [3].

This study evaluated a targeted *SMN1* genetic screening test to enable early and accurate differentiation between SMA and metabolic disorders

Methods. At the Institute of Mother and Child (IMC), we developed and validated a custom genetic screening test for SMA (Innovation Act no. 562/07.03.2024), designed to detect homozygous deletions of the *SMN1* gene. In parallel, an MLPA assay was implemented for diagnostic confirmation. The study included 96 symptomatic patients presenting with hypotonia and other features suggestive of SMA or metabolic disorders. Data was analyzed descriptively; categorical variables were expressed as frequencies and percentages.

Results. Application of the developed genetic screening test for spinal muscular atrophy were identified *SMN1* deletions consistent with SMA in 36 patients with overlapping manifestations (37.5%, 95% CI 27.8-47.9). The most frequent manifestations included generalized hypotonia (31.2%), severe motor delay (32.3%), recurrent respiratory infections (22.9%), and congenital or structural lung disease (10.4%) - features also commonly described in metabolic disorders. These clinical features reflect a predominantly neuromuscular pattern of involvement, consistent with disorders affecting lower motor neuron integrity and respiratory function, manifestations that are also commonly encountered in various metabolic disorders.

Conclusion. The implementation of a targeted genetic screening test for *SMN1* deletions in symptomatic infants enables early and accurate differentiation between SMA and metabolic disorders. This approach reduces the need for invasive investigations, accelerates diagnostic decision-making, and supports timely therapeutic intervention. Integrating molecular testing into the initial diagnostic workflow represents a pivotal step toward precision medicine in neonatal and pediatric care.

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References

1. Prior, T.W., Leach, M.E., Finanger, E.L. Spinal Muscular Atrophy. 2000 Feb 24 [Updated 2024 Sep 19]. In: Adam MP, Feldman J, Mirzaa GM, et al., editors. GeneReviews® [Internet]. Seattle (WA): University of Washington, Seattle; 1993-2025. Table 5. [Disorders to Consider in the Differential Diagnosis of Spinal Muscular Atrophy].
2. Qu, R., Yao, F., Zhang, X. et al. SMN deficiency causes pain hypersensitivity in a mild SMA mouse model through enhancing excitability of nociceptive dorsal root ganglion neurons. Sci Rep 9, 6493 (2019).
3. Deguise, M.-O.; Chehade, L.; Kothary, R. Metabolic Dysfunction in Spinal Muscular Atrophy. Int. J. Mol. Sci. 2021, 22, 5913. https://doi.org/10.3390/ijms22115913

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PP2.24

Diagnosis of congenital disorder of glycosylation (CDG)

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Introduction. Congenital Disorders of Glycosylation (CDG) are a heterogeneous group of rare, inherited metabolic diseases caused by defects in glycan biosynthesis and processing. Impaired glycosylation affects multiple organ systems, resulting in diverse clinical manifestations. Isoelectric focusing (IEF) of serum transferrin is an affordable and reliable diagnostic method for CDG. This study aimed to perform targeted screening for CDG by IEF among suspected patients in the Republic of Moldova.

Materials and methods. Serum samples from 319 patients aged 2 months to 15 years, clinically suspected for CDG, presenting with hypotonia, psychomotor delay, multisystem involvement, or dysmorphic features were analyzed. IEF was performed using the CSL-IEF chamber (Cleaver Scientific), Blue Power 3000 power supply, and SERVA reagents (Germany). Genetic testing for PMM2, MPI, ALG6, GALT, and ALDOB was conducted via Sanger sequencing on the ABI 3500Dx platform (Applied Biosystems).

Results. Implementation of IEF initially presented technical challenges, resolved through collaboration with RadboudUMC and SERVA. Screening of 319 samples from suspected patients identified abnormal transferrin profiles in nine patients(2.82%). To confirm and classify the specific types of CDG, molecular genetic analysis of glycosylation-related genes was performed(PMM2, MPI, ALG6, GALT, ALDOB). Pathogenic variants were detected in the GALT gene(GALT-CDG) in 6 patients(p.Q188R, p.E203L, p.K285N), in the ALDOB gene(ALDOB-CDG) in 2 patients(c.113-1_115del, p.A175D), and in the SSR4 gene(SSR4-CDG) in 1 patient(c.454A>G).

Conclusion. This study demonstrates successful implementation of IEF in Moldova as a diagnostic tool for CDG, enabling detection of glycosylation abnormalities and identification of specific CDG subtypes.

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PP2.25

Metabolomic evaluation for specific biomarkers in phenylketonuria

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Introduction. Phenylketonuria (PKU) is an inherited metabolic disorder caused by mutations in the *PAH* gene, leading to deficient phenylalanine hydroxylase (PAH) enzyme activity. This defect impairs the conversion of Phenylalanine (Phe) to Tyrosine (Tyr), causing systemic Phe accumulation. In the Republic of Moldova (incidence ~1:7,000), this neurotoxic accumulation leads to severe, irreversible intellectual disability if not detected by neonatal screening. The disease spectrum is wide, determined by over 3,370 *PAH* mutations. While management relies on a burdensome, lifelong low-Phe diet, and sometimes tetrahydrobiopterin (BH4) supplementation, this significantly decreases patients' quality of life. Consequently, research is focused on improving long-term monitoring and developing alternative therapies.

Materials and methods. This cross-sectional, observational study will investigate the relationship between *PAH* gene variants and specific metabolomic biomarkers in 60 genetically-confirmed PKU patients enrolled from Moldova's national screening program at the Institute of Mother and Child. Over one year, DBS, blood, and urine samples will be collected 1-4 times per month. A multi-platform analytical approach will be used:

1. **HPLC:** To quantify the full amino acid spectrum.
2. **1H-NMR Spectroscopy:** To analyze urinary organic acids and toxic Phe metabolites.
3. **PCR/Sanger Sequencing:** To identify specific *PAH* gene mutations.

The final objectives are to establish clear associations between genotypes and metabolomic phenotypes, develop a dedicated PKU biobank (serum, plasma, urine, DNA), and populate the National Registry for Rare Diseases with this comprehensive data.

Discussion and conclusion. This research leverages Moldova's comprehensive national PKU screening program (134 patients confirmed since 1989) to move beyond simple detection. By integrating advanced analytical methods, we aim to elucidate the complex relationship between a patient's genotype and their broader metabolomic profile. This is crucial, as HPLC data can help individualize diet therapy by accounting for Large Neutral Amino Acid (LNAA) transport, while 1H-NMR can quantify the specific toxic metabolite load.

We expect to identify novel biomarkers and generate clinical recommendations for adjusting diet therapy based on specific genotype-metabolome correlations. By characterizing the mutations and metabolic profiles specific to the Moldovan population, this work will contribute valuable local data to international repositories (e.g., BIOPKU) and the National Registry. The relevance of this research lies in its potential to significantly improve the diagnosis, long-term management, and treatment of PKU, ultimately enhancing patient quality of life.

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PP2.26

Implementation of primary HPV testing in cervical screening

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Introduction. Cervical cancer (CC) remains a major public health issue in the Republic of Moldova, ranking as the third most common malignancy among women. Human papillomavirus (HPV) infection is recognized as the primary etiological factor in the development of cervical cancer. HPV vaccination and cervical screening are two highly effective interventions that have the potential to eliminate cervical cancer entirely. The low effectiveness of the current cytology-based screening approach highlights the need to adopt more sensitive screening methods.

Objective. To assess the feasibility and clinical effectiveness of HPV testing as a primary cervical screening method in the Republic of Moldova, in comparison with the current cytology-based approach.

Materials and methods. A cross-sectional analysis of preliminary data from a feasibility study was conducted among women aged 30–65 years without known precancerous lesions, comparing primary HPV testing with conventional cytology. Women who tested positive for HPV types 16/18 were referred directly for colposcopy, whereas those positive for other high-risk HPV types were triaged using cytology.

Results. A high incidence of cervical cancer was identified among women aged 35–54 years, with the peak incidence (70.5%) observed in the 45–49 age group. Cytology did not contribute to a reduction in incidence and required frequent repeat testing. Within this population, a high detection rate of HPV 16/18–positive cases were observed, enabling direct referral to colposcopy and thereby shortening the diagnostic and intervention interval.

Conclusions. Primary HPV testing for cervical screening demonstrates enhanced early detection and improved efficiency by reducing the need for frequent repeat testing at short intervals. This primary screening method may prove effective for the Republic of Moldova; however, the occurrence of cervical cancer in HPV-negative women suggests the potential involvement of additional factors at the metabolic and/or genomic level.
Keywords: Cervical cancer, HPV testing, metabolism.

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PP2.27

Endocrino-metabolical features in childhood obesity

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Introduction. The prevalence of children overweight has steadily increased worldwide in recent decades. The situation is worring, as it puts its mark on both the child's current and future adult health. Excess weight involves multiple interactions between genetic, social, behavioral, metabolic, cellular and molecular factors that results in changes in energy balance. Hereditary intervenes through polygenic mechanism, being identified over 250 genes or chromosomal regions, influencing the general metabolism. Childhood obesity is associated with a number of metabolic abnormalities, such as dyslipidemia, insulin resistance and high blood pressure. Research on protein metabolism is of particular interest, especially the ratio of brached-chain amino acids serves as a predictor of the risk associated with childhood obesity. The concentrations of the amino acids cystine, glutamine, glycine, histidine, isoleucine, leucine, lysine, tryptophan and valine reveal a steadily increasing during childhood and adolescence. Five amino acids aspartic acid, citrulline, glutamic acid, serine and taurine maintain a constant concentration throughout childhood. In obese children, lower levels of free amino acids are determined compared with those with normal weight. The change in the ratio of branched-chain amino acids in obesity is determined by the changed activity oh the mTorc1complex, which contributes to decreased insulin sensitivity and accumulation of the toxic metabolites, which can induce mitochondrial dysfunction, kinase activation and pancreatic cell damage. Decreased insulin sensitivity is associated with lower concentrations of 2-ketobutyrate, citrate and 3-hydroxybutyrate. The analysis of the ratio of branched-chain serves as a predictor of the risk associated with child obesity.

Material and methods. In the order to describe the metabolomic features 120 obese children have been selected for the research and there were collected the materials (blood, serum, plasma, DBS, DNA and urine) for analysis of amino acids (by HPLC), urinary organic acids (by NMR Spectroscopy) and molecular-genetic analysis (by PCR) which will be done. These data will be analysed before diet and after its establishing 2-6-12 monts later.

Results and conclusion. A such approach will provide the data on biomarkers specific for childhood obesity, their particularities and prediction of clinical evolution.

Keywords: childhood obesity, amino acids, insulin sensitivity.

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PP2.28

Interplay between the microbiome and metabolome in the gastric precancerous transformation

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The gastric precancerous cascade, progressing from chronic active inflammation toward atrophic gastritis, intestinal metaplasia, dysplasia, and ultimately gastric cancer, is shaped by a complex interaction between microbial and metabolic factors. Helicobacter pylori represents the central microbial driver, initiating chronic inflammation that alters the gastric microenvironment and triggers profound metabolic reprogramming of epithelial and immune cells. This interplay between the microbiome and metabolome is pivotal in determining whether early lesions regress, persist, or progress toward malignancy.

The microbiome exerts its influence not only through persistent colonization and mucosal injury but also through the modulation of host metabolic pathways. H. pylori–induced changes in nitric oxide (NO) metabolism, pepsinogen secretion, and gastrin-17 (G-17) regulation highlight the metabolic consequences of microbial persistence. Our study demonstrated that serum biomarkers, particularly PG-I, the PG-I/PG-II ratio (PGR), and G-17, decline progressively with worsening histological lesions, while NO levels increase both in serum and gastric juice, reflecting ongoing inflammation and mucosal atrophy. These findings align with the OLGA and OLGIM staging systems, underscoring the value of integrated microbiome–metabolome assessment in risk stratification.

The metabolomic perspective provides additional insight into the functional activity of the gastric mucosa beyond morphological evaluation. Low PG-I and reduced PGR, as hallmarks of advanced atrophy, correlate with microbial-induced impairment of secretory capacity. Similarly, elevated NO production represents a metabolic footprint of sustained oxidative stress driven by H. pylori–mediated inflammation. Together, these metabolic signatures serve as non-invasive surrogates of mucosal damage and precancerous progression, complementing traditional histology and endoscopy.

Importantly, the limitations of invasive diagnostic approaches, such as magnification endoscopy and targeted biopsies, highlight the urgent need for combined microbial and metabolic biomarkers in clinical practice. The integration of microbiome profiling with serological and metabolomic markers holds promise for earlier, less invasive detection of precancerous lesions and improved monitoring of high-risk patients.

In conclusion, the gastric precancerous transformation reflects a dynamic crosstalk between the microbiome and metabolome. H. pylori infection remains the keystone initiator, but its pathogenicity is mediated through metabolic alterations that progressively impair gastric mucosal structure and function. Future approaches should focus on multi-omics integration, combining microbial and metabolic signatures to refine risk prediction and develop personalized surveillance strategies aimed at reducing gastric cancer burden.

Keywords: Helicobacter pylori, microbiome, metabolome, gastric precancerous lesions, biomarkers.

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PP3.1

Laser-fabricated bioactive thin films: a versatile platform for advanced biomedical coatings

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Surface coatings play a critical role in enhancing the biological performance of implants and wound interfaces, offering protection, bioactivity, and targeted therapeutic functionality.
The integration of laser techniques with bioactive material design offers a highly versatile platform for creating next-generation wound dressings, implant coatings, and scaffolds for soft and hard tissue regeneration. The use of Matrix-Assisted Pulsed Laser Evaporation allows for the deposition of bioactive thin films with nanoscale precision and minimal thermal damage, crucial features for preserving the functional properties of delicate biomolecules. Moreover, the versatility of the laser-based approach enables the incorporation of antimicrobial agents into the film matrix, supporting multifunctional coatings which can be tailored to specific clinical needs.

The physical-chemical characterization of the coatings was carried out using techniques such as Scanning Electron Microscopy and Atomic Force Microscopy to evaluate surface morphology and roughness, Contact Angle measurements to assess wettability, and Fourier Transform Infrared Spectroscopy to confirm the chemical integrity and functional group preservation of the deposited materials.

Biological in vitro assays confirm the functionality of the thin films, showing that they support key processes involved in tissue repair and regeneration.

Laser-fabricated bioactive coatings demonstrate strong potential as versatile and effective platforms for a wide range of biomedical applications.

Acknowledgements
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PP3.2

From precipitate to thin films: Unveiling the structure of polydopamine coatings by solid-state NMR

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Abstract

Despite extensive studies, the atomic-scale structural differences between polydopamine (PDA) coatings and bulk PDA precipitates remain poorly understood. This gap hinders a comprehensive explanation of PDA's adhesion mechanisms and limits the design of PDA-based surfaces and interfaces. To address this challenge, a two-pronged approach was employed: (i) selective deuteration of the catechol ring in dopamine to synthesize deuterated PDA structures with varying thicknesses deposited on SiO_2 nanoparticles, and (ii) advanced solid-state NMR techniques—including ^{2}H solid echo and $^{13}C/^{15}N$ cross-polarization—combined with electron microscopy for structural characterization. Our results reveal that nano-sized PDA coating layers are structurally similar to bulk PDA. However, for films thinner than 5 nm, we identified distinct surface-specific features: an enrichment in monomeric units bearing aliphatic carbons and protonated amine groups ($-NH_3^+$) compared to the underlying oligomer layers. These findings offer new insights into the molecular organization at PDA interfaces and contribute to a deeper understanding of its adhesion behavior [1].

Acknowledgments

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References

1. X. Filip, A. Simion et all., Applied Surface Science 649(2007):159190, DOI: 10.1016/j.apsusc.2023.159190

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PP3.3

Effects of incorporating a 3D coordination polymer with siloxane fragments on the properties of silicone

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A three-dimensional coordination polymer, $[Cd(Cx)(AzPy)\cdot 1.85H_2O]_n$ (Compound 1) obtained by the reaction of 1,3-bis(carboxypropyl)tetramethyldisiloxane (Cx), 4,4′-azopyridine (AzPy) and cadmium perchlorate was incorporated in two mass fractions (5 and 20 wt%) into a silicone matrix consisting of high molecular weight PDMS. The resulted composites PDMS-C1-5 and PDMS-C1-20, processed into films and stabilized by cross-linking with TEOS in the presence of DBTDL, were investigated in terms of morphology, as well as mechanical and electrical properties. SEM analysis in section of the films fractured in liquid nitrogen (Figure 1a) reveals the presence of relatively uniform, in size and distribution, of Compound 1 particles within the silicone matrix. Mechanical behavior was evaluated by recording stress–strain curves (Figure 1b). The results showed that introducing Compound 1 into the PDMS matrix increases Young's modulus, tensile strength, and elongation at break compared to the reference sample, PDMS-0, without filler. The reinforcing role of Compound 1 is further confirmed by the toughness values (UTT), which are at least three times higher for both composites compared to the reference. All samples exhibit large elongations at break, ranging from 1019% for PDMS-0 to 1267% for PDMS-C1–5. Dielectric measurements of the composites (Figure 1c,d) indicate that polarization phenomena at low frequencies are strongly reduced, resulting in relatively low and stable permittivity values across the investigated frequency range. In contrast, dielectric losses are lower and decrease more significantly with frequency above 10 Hz for the composites, compared to PDMS-0. Along with the very low conductivity values, these findings demonstrate the strong insulating character of Compound 1. Thus, when incorporated as a filler, it acts as an effective mechanical and dielectric reinforcing agent for silicone elastomers. The high dielectric strength is particularly relevant for applications in dielectric elastomer transducers. Theoretical calculations based on the mechanical and dielectric parameters confirm that these silicone composites are suitable for electromechanical transducers operating in generator mode [1].

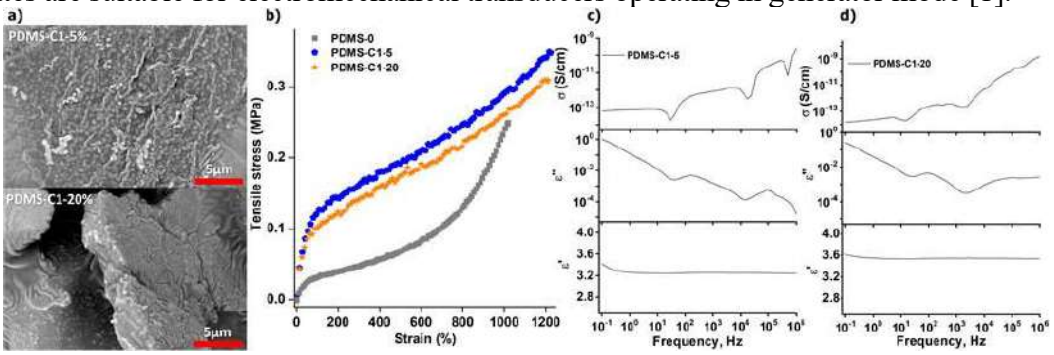

Figure 1. a) SEM images in cross-section of PDMS-C1 composite films; b) Stress-strain curves of the prepared silicone films; Dielectric spectra for: c) PDMS-C1-5; d) PDMS-C1-20.

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Reference

1. A.-C. Stoica et al., Reactive and Functional Polymers, 2024, 197, 105876.

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PP3.4

Hybrid cellulose nanofiber–PVTMS aerogels: ultralight, porous, and floatable materials

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Aerogels combine ultralight weight, high porosity, large surface area, and excellent stability, making them ideal for advanced applications such as insulation, energy storage, and catalysis. Our purpose is to use macroporous aerogel matrices as supports for photocatalyst immobilization to prevent leaching, enhance loading capacity, and improve mass transfer. Unlike dense films or submerged polymer–photocatalyst composites, our strategy is to create floatable substrates that remain at the air–water interface, maximizing solar exposure, oxygen availability, and overall photocatalytic efficiency.

Cellulose nanofibers (CNFs), with diameters of 4–100 nm and micrometer-scale lengths, are attractive aerogel precursors owing to their high crystallinity, strength, low density, and tunable surface chemistry, which facilitate the formation of ultralight, porous networks. Their mechanical stability can be further enhanced through chemical crosslinking, which also enables control over surface wettability.

In this work, CNFs were hybridized with poly(vinyltrimethoxysilane) (PVTMS), whose controlled hydrolysis and condensation produced silanol groups (Si–OH) that bonded strongly with the CNF network, reinforcing the structure and yielding robust, floatable hybrid aerogels. Cellulose nanofibers (CNFs) for the aerogel network were prepared in our laboratory using a combination of alkaline–acid hydrolysis, ultrasonication, and TEMPO-mediated oxidation. To assess the influence of cellulose source and polymer chain length, CNFs were extracted from materials with different degrees of polymerization (DP): cotton linters (CL, DP = 465), microcrystalline cellulose (MCC, DP = 140), alpha cellulose (α-CEL, DP = 950), and eucalyptus cellulose (EYPT, DP = 2742). Poly(vinyltrimethoxysilane) (PVTMS) was synthesized by free radical polymerization of vinyltrimethoxysilane and subsequently employed to fabricate ultralight, highly porous, and floatable aerogels. The hybrid aerogels were characterized by FTIR spectroscopy and SEM/EDX to investigate CNF–PVTMS interactions, morphology, and structural uniformity. In addition, it was demonstrated enhanced moisture stability and improved structural integrity of the synthesized aerogels.

Acknowledgements
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PP3.5

Carbonaceous composites from plant materials: production and characterization

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Activated carbon obtained via hydrothermal synthesis and fluidized-bed activation exhibits well-developed porosity and high specific surface area, which are essential for adsorption and catalytic applications. The hydrothermal method converts biomass into carbonaceous materials rich in functional groups [1], while fluidized-bed activation ensures a uniform distribution of micropores and mesopores through efficient contact with activating agents. This combination results in carbon composites with surface areas up to 2500 m^2/g, favorable for water purification and catalytic processes [2].

The present study examines the physico-chemical characteristics and surface chemistry of carbon composites obtained via hydrothermal synthesis (impregnated with iron, cobalt, nickel, copper, and manganese salts) and fluidized-bed activation, using SEM-EDX analysis and determination of the pH_{pzc}.

Morphological analysis of the laboratory-prepared activated carbons (ACCN-1, ACCN-Co1, ACCN-Mn1, ACCN-Cu1, ACCN-Ni1) demonstrated the presence of cobalt, manganese, copper, and nickel ions on the activated carbon surfaces in the following proportions: 2.85%, 1.22%, 4.15%, and 0.80%. The acid–base properties of the activated carbons were studied through pH-metric titrations to determine the point of zero charge (pH_{pzc}). For the initial activated carbon ACCN-1, the surface charge is zero within the pH range of 5.02–9.30, and the pH_{pzc} value obtained by extrapolation is 7.4. For samples impregnated with cobalt, nickel, copper, and manganese, the pH_{pzc} values range from 7.9 to 8.4.

Impregnation with transition metal ions led to an increase in pH_{pzc} values, indicating a reduction in the acidic character of the surface and a potential improvement in the adsorption of anionic species.

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References

1. Jiang, X., Shi, G., Wang, G. et al. A hydrothermal carbonization process for the preparation of activated carbons from hemp straw: an efficient electrode material for supercapacitor application. Ionics 25, 3299–3307 (2019). https://doi.org/10.1007/s11581-019-02850-8
2. Muratova, N.S., Is'emin, R.L., Melezhik, A.V. et al. Results of Chemical Activation of Biochar Obtained by the Method of Accelerated Hydrothermal Carbonization of Sewage Sludge. J Eng Phys Thermophy 94, 1557–1562 (2021). https://doi.org/10.1007/s10891-021-02436-0

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PP3.6

Obtaining activated carbon by chemical method by utilizing local waste

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The Republic of Moldova offers favorable conditions for walnut production, and the walnut sector presents significant opportunities for valorization. Walnut shells, a by-product of this industry, are an abundant and underutilized resource with potential applications in various industrial and environmental processes [1]. Activated carbon derived from walnut shells demonstrates high efficiency in water treatment, removing pollutants such as heavy metals, dyes, and volatile organic compounds. Its high adsorption capacity results from the porosity and functional groups introduced during activation, making it an eco-friendly and sustainable alternative to conventional purification materials [2].

Chemical method of activation using citric acid is an environmentally friendly and biocompatible approach for converting walnut shells into activated carbon. The raw materials were crushed and sieved to a size of between 2÷4 mm, this fraction was used for the preparation of activated carbon. The process involved impregnating the shells with an aqueous citric acid solution, followed by carbonization at moderate temperatures (~500 °C for 2 h) under an inert atmosphere. Citric acid acts as an activating agent, generating surface functional groups that enhance adsorption performance (Fig. 1).

Thus, the abundant waste of walnut shells in Republic of Moldova can be efficiently transformed into high-performance activated carbon via citric acid activation, yielding a porous material with tailored surface chemistry for effective removal of water pollutants. The next steps will include the physico-chemical characterization of activated carbon obtained by different methods.

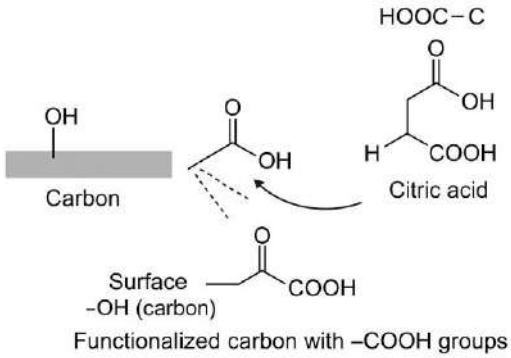

Figure 1. Functional groups on the surface of activated carbon by activation with citric acid

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References

1. Yaman, M. and Demirel, M. H. (2020). Synthesis and characterization of activated carbon from biowaste-walnut shell and application to removal of uranium from waste. *Pollution*, *6*(4), 935-944. doi: 10.22059/poll.2020.303546.828
2. Segovia-Sandoval, S. J., et al. (2018). *Walnut shell treated with citric acid and its application as biosorbent in the removal of Zn(II). Journal of Water Process Engineering, 25, 45-53.* https://doi.org/10.1016/j.jwpe.2018.06.007

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PP3.7

Synthesis, crystal structure, and intermolecular interactions evaluation via Hirshfeld surface analysis of a copper(II) complex with 3-pyridine aldoxime

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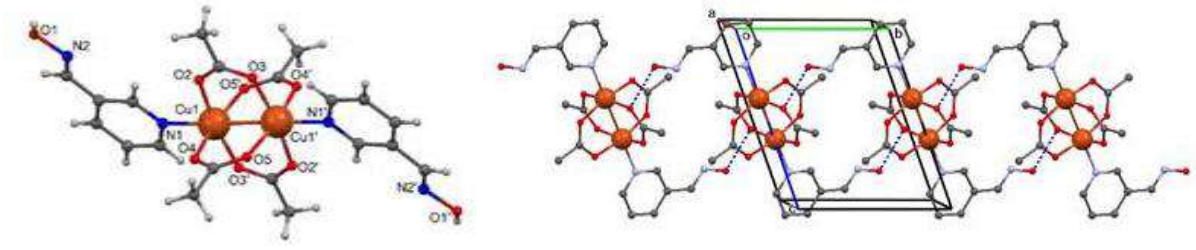
The design and synthesis of transition metal coordination complexes involving bioactive ligands, such as 3-pyridinealdoxime (3-pyaoH), may impart antimicrobial or enzyme-inhibitory properties to these complexes, thereby expanding their potential applications in bioinorganic and medicinal chemistry [1].

Herein, we report the crystal structure of a new Cu(II)/3-pyridine aldoxime complex, $[Cu_2(MeCO_2)_4(3\text{-pyaoH})_2]$, obtained from the reaction of copper(II) acetate monohydrate with 3-pyaoH in a MeOH/DMF solvent mixture. Additionally, we investigate the intermolecular interactions present in the structure.

The title compound represents a new member of Cu(II) carboxylate complexes with a *paddle-wheel* structure [2]. It crystallizes in the triclinic *P*-1 space group with unit cell parameters: a=7.9106(4), b=8.3214(7), c=10.1943(9) Å, α=69.788(8), β=88.9(6), γ=86.555(5)°, and V=628 Å^3. The two Cu(II) centers are bridged by four *syn, syn-η1:η1:μ* $MeCO_2^-$ ligands, forming the dinuclear core. Each Cu(II) ion adopts a square-pyramidal coordination geometry in which the apical position is occupied by the pyridyl nitrogen atom of a monodentate 3-pyaoH ligand. The Cu···Cu separation is 2.6439(5) Å. Each Cu(II) atom is displaced by 0.207Å from its least-squares basal plane toward the coordinating pyridyl nitrogen atom. The mean Cu–O(carboxylate) bond length is 1.9715(2) Å. In the crystal structure, the dinuclear molecules are interconnected through hydrogen-bonding interactions, forming supramolecular ladder-like chains that extend along the crystallographic *b*-axis. Both oxime groups act as hydrogen bond donors towards the carboxylated oxygen atoms, forming hydrogen bonds, O1–H...O5 = 2.752(3)Å. The distribution of intermolecular interactions was evaluated using Hirshfeld surface analysis, which reveals that H···H contacts are the predominant interactions contributing to the stabilization of the crystal packing.



a **b**

Fig.1. Molecular structure with partial labeling (**a**) and fragment of supramolecular chain (**b**)

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References

1. K.F. Konidaris, R. Papi, E. Katsoulakou, C.P. Raptopoulou, D.A. Kyriakidis, and E. Manessi-Zoupa. Synthesis, Crystal Structures, and DNA Binding Properties of Zinc(II) Complexes with 3-Pyridine Aldoxime. Bioinorganic Chemistry and Applications, 2010, 1-7.
2. L.Croitor, E.B. Coropceanu and M.S. Fonari. Anion–pyridine-n-oxime interplay to control metal–metal separations in a series of Cu(II) coordination polymers. CrystEngComm, 2022,24, 6146-6154.

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PP3.8

Two Eu(III) compounds with biologically relevant triimidazo[1,2-*a*:1′,2′-*c*:1″,5″-*e*][1,3,5]triazine luminophore

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Lanthanides have diverse applications spanning from contrast agents in Magnetic Resonance Imaging (MRI) to luminescent probes for bioimaging and biosensing [1]. In this regard, europium complexes can be used as molecular thermometers to measure temperature with high sensitivity in tiny spaces like living cells or microfluids [2]. In continuation of our previous research that revealed the excitation-dependent and temperature-dependent photoluminescence (PL) of Eu(III) complexes with pyridine-functionalised TTs (where TT is a triazine-based scaffold, namely triimidazo[1,2-*a*:1′,2′-*c*:1″,2″-*e*][1,3,5]triazine) [3], herein we report two new Eu(III) crystalline materials with its positional isomer, [1,2-*a*:1′,2′-*c*:1″,5″-*e*][1,3,5]triazine (iso-TT). Cocrystal $[Eu(NO_3)_3(H_2O)_4]\cdot(\text{iso-TT})_2\cdot(H_2O)$ (**1**) and mononuclear complex $[Eu(NO_3)_3(H_2O)_3(\text{iso-TT})]$ (**2**) were prepared by solvothermal reaction of europium nitrate with iso-TT. **1** crystallizes in the *Pbcn* orthorhombic space group with $[Eu(NO_3)_3(H_2O)_4]$, iso-TT and water molecules interconnected via OH···O, OH···N, and CH···N hydrogen bonds. The crystal packing is built of the alternating inorganic/organic H-bonded motifs (Fig. 1, left) where triazine molecules form stacking columns with the meaningful molecular overlap. **2** belongs to the monoclinic $P2_1/c$ space group and reveals the direct Eu-N(iso-TT) coordination bond (Fig. 1, right). The distribution of intermolecular interactions in **1** and **2** was evaluated using Hirshfeld surface analysis.

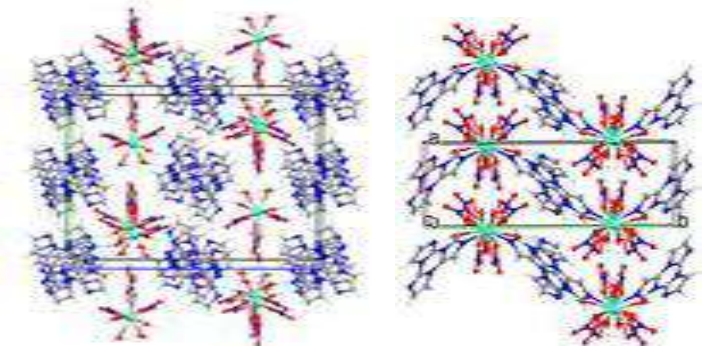

Figure 1. Crystal packing in **1** (left) and **2** (right).

The photoluminescent behavior and its correlation with the crystal structure is currently under investigation for both compounds.

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References

1. C. Alexander, Z. Guo, P. B. Glover, S. Faulkner, Z. Pikramenou Chem. Rev. 2025, 125, 2269−2370,
2. A. Carlotto, L. Babetto, S. Carlotto, M. Miozzi, R. Seraglia, M. Casarin, G. Bottaro, M. Rancan, L. Armelao ChemPhotoChem, 2020, 4, 674-684
3. V. Ch. Kravtsov, V. Bold, N. Siminel, Y. Chumakov, Maria Gdaniec, E. Lucenti, D. Malpicci, D. Maver, M. S. Fonari Cryst. Growth Des. 2024, 24, 4875−4883

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PP3.9

Structural diversity of Co(II, III) compounds assembled from pivalate and hexamethylenetetramine ligands

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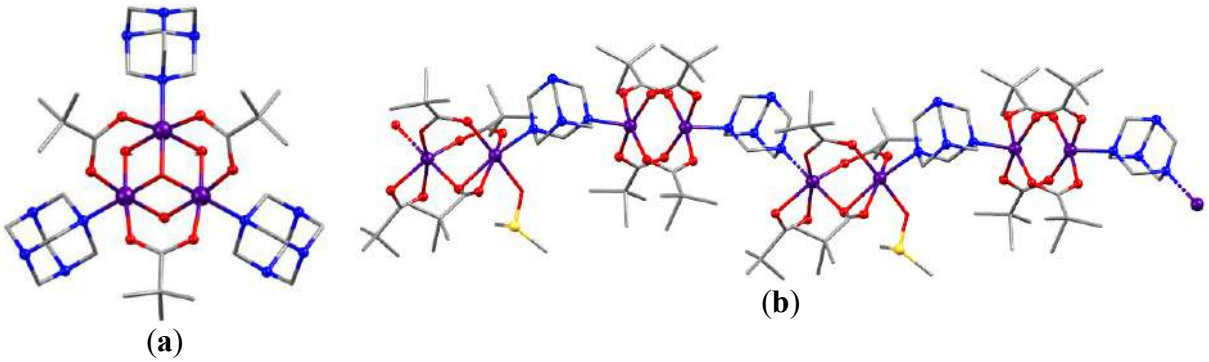
Hexamethylenetetramine (hmta), also known as urotropine or tetraazaadamantane, is a polycyclic, cage-like ligand in which four nitrogen atoms occupy the vertices of a tetrahedral framework. The tetrahedral arrangement of nitrogen lone pairs makes hmta an appealing candidate as a tetrahedral building block in supramolecular architectures. Importantly, this structural versatility exerts a pronounced influence on the resulting properties, such as porosity, stability, magnetism, and catalytic activity, enabling the targeted design of materials with diverse applications, including medical uses. In this context, two compounds have been synthesized by the reaction of Co(II) pivalate with hmta in dmso using ultrasonic irradiation: μ_3-oxo trinuclear $[Co_3O(OH)_3(piv)_3(hmta)_3](piv)\cdot$dmso (**1**) cluster and 1D coordination polymer $\{[Co_2(piv)_4$-hmta-$[Co_2(piv)_4(dmso)]\}_n$ (**2**). X-ray structural analysis shows that the $\{Co_3\}$ core in **1** consists of three Co(III) atoms, which are interconnected by three bridging pivalate ligands and three μ_2-hydroxo and μ_3-oxo groups. The structure shows that the hmta ligands coordinate through a N atom to a Co atom and extend to the exterior, while the Co atoms are held together by the central polyoxo framework at Co…Co distances of 2.736–2.745 Å. The coordination polyhedron of the each Co(III) ion adopts a distorted NO_5 octahedral surrounding formed by μ_3-O, two OH^- groups, two O atom from piv^-, and one N atom from hmta (Fig. 1a). Polymeric compound **2** reveals two different dinuclear Co(II) fragments, which are connected by a hmta molecule and generate a coordination extension in a 1D chain architecture (Fig. 1b). In one of these fragments, the Co atoms are coordinated by eight O atoms from four carboxylate groups, which act in a bridging coordination mode, providing a Co…Co separation of 2.690 Å. In the other fragment, two pivalate groups bridge the Co atoms, while two additional pivalates coordinate in a chelating manner, resulting in a Co…Co separation of 3.413 Å. Moreover, one dmso molecule is also coordinated. All Co atoms display a distorted NO_5 octahedral environment in **2**.



(**a**) (**b**)

Fig. 1. Structure of cluster **1** and the fragment of 1D chain in **2**.

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PP3.10

The influence of selenium oxide, cerium oxide and molybdenum oxide on some properties of apatite-wollastonite glass ceramics

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The research aims to obtain and characterize a biomaterial based on apatite-wollastonite glass ceramics with various additives (selenium oxide, cerium oxide, and molybdenum oxide) for potential use in medical applications such as post-cancerous bone reconstruction. Throughout the study, the resulting materials were tested for morphological, mechanical, ceramic, and biological properties to assess their suitability for such an application.

Regarding the glass ceramic materials, apatite-wollastonite glass ceramic compositions were synthesized via the sol-gel method, while the additives were incorporated in a proportion of 5%wt. After homogenizing the specific precursors, the gels were then dried, and the powders obtained were calcined at temperatures established by a complex thermal analysis (DTA+TG). After sintering at different temperatures, the phase composition was determined by X-ray diffraction. Also, the ceramic properties (open porosity and relative density), the mechanical properties (compression strength and elasticity modulus), structural morphology (determined by scanning electron microscopy – SEM), as well as biological behaviour (pH variation and the phosphates deposition upon immersion in SBF for 28 days and the effect the material has on AFSC cell cultures) were determined.

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PP3.11

Compatibility assessment and characterization of non-hydraulic binder mortars in heritage church structures

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Historic churches were often built with traditional mortars based on non-hydraulic lime binders, which harden through carbonation and ensure compatibility with natural stone and brick. Over time, environmental factors and restorations can alter their composition. Analytical methods such as DGA (TG/DTG) and SEM-EDS (Figure 1) are essential to assess thermal behavior, mineral composition, and binder type, confirming the non-hydraulic nature of the material and guiding compatible conservation practices.

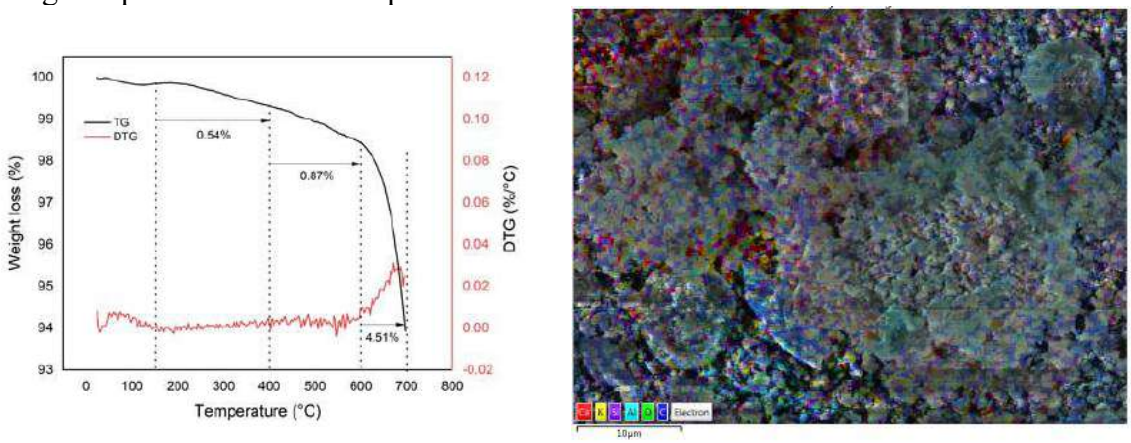

Figure 1. DGA (TG/DTG) and SEM-EDS characterization of mortar collected from the historic church walls.

The DGA (TG/DTG) analysis reveals a gradual and limited weight loss below 700 °C, indicating the absence of significant decomposition reactions associated with hydration products. Minor mass decreases below 600 °C correspond to the evaporation of physically adsorbed and weakly bound structural water, while a more pronounced loss above 600 °C is attributed to decarbonation processes. The lack of distinct exothermic or sharp decomposition peaks confirms that the material does not form hydraulic compounds upon contact with water. These thermal features classify the analyzed sample as a non-hydraulic binder, whose setting and hardening occur primarily through carbonation. Complementary SEM-EDS analysis supports these results, showing a heterogeneous microstructure dominated by Ca-, Si-, and Al-rich phases within a carbonaceous matrix. Elemental mapping indicates calcium and silicon are closely associated with carbon, suggesting the presence of calcium carbonate and amorphous silicate phases rather than hydrated products. The absence of C–S–H gel or other hydration-related morphologies further confirms that the cohesion of the material is governed by carbonation reactions, validating its characterization as a non-hydraulic binder.

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PP3.11

Antimicrobial chitosan-based cross-linked networks with re-mendable thermoresponsive properties

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The utilization of biomass resources for producing natural polymeric materials is highly demanding due to its potential to reduce solid waste generation and dependence on fossil resources. This study explores the development of thermoreversible bio-based cross-linked polymeric networks, designed as films, by leveraging the properties of polysaccharides and vegetable oils through the Diels-Alder reaction. Chitosan (CS) was first grafted with furyl groups and subsequently cross-linked with maleimide-functionalized castor oil. The effects of varying degrees of substitution of CS and different furyl-to-maleimide ratios on material properties were investigated. The resulting crosslinked networks exhibited enhanced thermal stability compared to unmodified CS. DSC analysis confirmed the retro Diels-Alder reaction occurring between 103–115 °C. Notably, the reproducibility of the retro Diels-Alder process in DSC experiments was demonstrated for the first time, marking a significant step in understanding CS-based systems. This advancement highlights their potential for applications requiring reversible cross-linking, such as responsive or recyclable materials. Additionally, the networks exhibited strong antimicrobial activity, achieving up to 100% inhibition of E. coli and S.aureus, depending on the degree of substitution of CS and the furyl-to-maleimide ratio, which recommend their potential application as antimicrobial coatings.

Acknowledgments
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PP4.1

Hydrogen peroxide-induced photolysis of vitamin B_9 in aquatic systems

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The aim of this work is to evaluate the induced photolysis of vitamin B_9 in natural waters on model systems. To identify the kinetic laws of induced photolysis of vitamin B_9 (folic acid) in aquatic systems, the following system was modeled: $B_9–H_2O_2 –h\upsilon$. In this research, the solar simulator Model Oriel 9119X (SS) and the DRT-400 lamp were used as irradiation sources. Based on the practical results, the kinetic parameters of induced photolysis (in the presence of hydrogen peroxide as a source of OH radicals) were determined (Table 1).

Table 1. Kinetic parameters of the vitamin B_9 induced photolysis with H_2O_2 [*own data*]

Parameter / Irradiation source	$K \cdot 10^5$, s^{-1}	$\tau_{1/2}$	The reaction rate equation
Solar simulator	$1{,}27 \cdot 10^{-5}$	15 h 10 min 59 s	$W = K \cdot [AF]^{0.5} \cdot [H_2O_2]^{0.4}$
DRT-400 lamp	$8{,}59 \cdot 10^{-4}$	1 h 24 min 19 s	$W = K \cdot [AF]^{0.4} \cdot [H_2O_2]^{0.5}$

In previous studies, it was established that under conditions typical of natural aquatic systems, where vitamin B_9 concentrations are very low (10^{-9} – 10^{-8} M) and solar radiation is affected by weather forecasts, direct photolysis occurs at very low rates and can therefore be considered negligible. However, when hydrogen peroxide is introduced into the system, the degradation rate of vitamin B_9 increases of 1.5-10.0 times, compared to direct photolysis. This is attributed, on the one hand, to the formation of $^{\bullet}OH$ through the photodissociation of hydrogen peroxide. On the other hand, evidence suggests that vitamin B_9 contributes to the regeneration of additional radicals in the system, further accelerating its own degradation. When comparing the results obtained for systems irradiated under SS with those irradiated using the DRT-400 lamp, it is observed that the reaction rates under SS are approximately 5–6 times lower. The DRT-400 lamp's emission spectrum overlaps more effectively with the absorption spectrum of vitamin B_9 and hydrogen peroxide, causing this difference. Consequently, a greater concentration of $^{\bullet}OH$ is generated in the system. Kinetic analysis revealed that the individual reaction orders of the substrate and hydrogen peroxide are fractional. Mechanistically, this behavior suggests a competition between two concurrent processes, with their relative contributions depending on the concentrations of the reactants and the nature of the irradiation source. Based on the overall reaction order, it was determined that the induced photolysis of vitamin B_9 follows apparent first-order kinetics. The effective rate constants were calculated to be $8.59 \cdot 10^{-4}$ s^{-1} for systems irradiated with the DRT-400 lamp and $1.27 \cdot 10^{-5}$ s^{-1} for systems irradiated under SS. Thus, the effective rate constant under DRT-400 lamp irradiation is an order of magnitude higher than that under SS, and the corresponding half-life is approximately ten times shorter.

Thus, under natural water conditions, the half-life of vitamin B_9 during induced photolysis is 15 h 10 min 59 s, indicating that the substrate degradation proceeds relatively slowly. This suggests a high stability of vitamin B_9, which is essential for the survival of hydrobionts. Also, the presence of vitamin B_9 has a positive impact on the self-purification processes of natural waters. At the concentrations typically found in aquatic environments in the presence of H_2O_2 and solar radiation, vitamin B_9 will contribute to the regeneration of an additional amount of $^{\bullet}OH$, thereby enhancing the oxidative capacity of the system.

Acknowledgements: The results have been obtained in the framework of the project 010603 – Advanced research in computational and ecological chemistry, identification of technological procedures for treatment, formation of water quality and quantity, Institute of Chemistry of the Moldova State University.

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PP4.2

Eco-Efficiency of caffeine production methods

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Caffeine is a naturally occurring compound of plant origin, classified as a phytochemical, and is widely utilized in the food, pharmaceutical, and cosmetic industries. The specialized literature describes several methods for obtaining caffeine, either through extraction from natural sources or via chemical synthesis. These methods typically yield satisfactory amounts of the final product; however, they are also associated with various losses throughout most phases of the production cycle. Such losses include unconverted raw materials, solvent and energy consumption, and the generation of solid, liquid, or gaseous waste.

These inefficiencies highlight the potential for improving the eco-efficiency of industrial caffeine production by preventing or at least partially reducing such losses. This approach aligns with modern principles of resource efficiency and sustainable industrial practice. In this context, a comparative assessment was undertaken to evaluate the material, energy, and waste or pollutant flows associated with various known methods of caffeine production. The evaluation was based on key environmental and efficiency indicators, including *Life Cycle (LC) analysis*, *Atom Economy (AE)*, *Specific Waste Generation (SWG)*, and *Carbon Footprint (CF)*. The aim of the analysis was to identify specific stages in the technological process and life cycle phases that contribute to economic and ecological inefficiencies.

The production processes examined included the method of sublimation and extraction from plant material, particularly tea leaves, using water and dichloroethane, as well as two synthetic approaches, one based on uric acid and the other on 8-methylcaffeine. The life cycle assessment revealed multiple environmental impact categories associated with caffeine production. These include carbon dioxide emissions, solvent consumption, wash water discharges, solid and gaseous waste generation, and noise pollution originating from production facilities and the transportation of raw materials and finished products.

The atom economy was calculated to be 35% for the synthesis of caffeine from uric acid and 41% for synthesis from 8-methylcaffeine, both indicating a relatively low recovery rate of input substances and, consequently, high levels of production waste. The specific waste generation values, 4 for the uric acid method and 6 for the 8-methylcaffeine method, further classify these synthetic approaches as low in eco-efficiency.

While the extraction method from tea leaves avoids synthetic precursors, its ecological value is reduced due to the number of stages involved (four), the extended duration of the extraction process, the use of multiple materials (seven in total), a high specific waste value (four), and significant indirect greenhouse gas emissions. Nevertheless, one viable strategy for enhancing the eco-efficiency of this method could be the replacement of the two solvents currently used water and dichloroethane with a single, more environmentally friendly alternative.

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PP4.3

Determination of humic substances content in the wastewater of the treatment facilities of Cricova, Republic of Moldova

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Recently, the Republic of Moldova is facing an acute water shortage not only in terms of drinking water, food and even more so irrigation needs. Increasingly frequent periods of drought require us to search for new possibilities to replace river and lake water with water from other alternative sources to support the productivity of agricultural crops, irrigation. A considerable source could be water from wastewater treatment technologies (Biological wastewater treatment plants - WWTP). Wastewater treatment from urban and rural centers with state-of-the-art technologies makes it possible to obtain water of a quality suitable for irrigation of agricultural crops, which depend on many indicators, including biogenic elements (organic carbon, nitrogen and phosphorus) but also the content of humic substances (HS) that have an effect on improving irrigable soils. Therefore, monitoring their content for the purpose of use in this regard is important. The water flowing from WWTP Cricova into the natural effluent contains less than 18 mg/L of total nitrogen N and 6 mg/L of total phosphorus P. For the future, it is assumed that water purification will improve with regard to these indicators. Thus, the water from the technological activity of WWTP Cricova can be a source of support for agricultural crops with N and P without causing pollution of the irrigated watershed. As a result of the purification process, HS are generated and migrate with both natural waters and wastewater. In the final treatment stage, the water is discharged into rivers or other water bodies and continues to participate in the exchange of substances, so monitoring the HS content is of great importance, as they are a constituent part of soils, activated sludge and underwater sediments. HS further participates in the formation of humic acids, the most valuable component of soils.

Previously, we developed a spectrophotometric method for determination of water-soluble HS (Patent 4305 MD. Publication data: 2014.09.30.). The method was based on the interaction of HS with the basic dye methylene blue (MB). HS were extracted with methanol from the dry residue. The dry residue of the methanol extract was dissolved in distilled water, and an aqueous solution of MB was added to it. After 20 min, the original solution and the solution with the formed associate "HS - MB" were photometrically measured at a wavelength of 609-611 nm. Spectra were recorded using a Lambda 25 spectrophotometer. The content of HS (C_{HS}, mg/L) was calculated based on the difference in light absorption ΔA at the maximum between the solutions of MB and the MB associate with HS. The determination error of HS did not exceed 5%. We obtained the following results for determination the content of HS (C_{HS}, mg/L) in wastewater at different stages of treatment in the wastewater treatment facilities of the town of Cricova (Republic of Moldova): 1) Effluent, discharge to river, sample from 04/08/2024, 1.322 mg/L; 2) Outlet, 1st line, sample from 04/17/2024, 1.787 mg/L; 4) Outlet, 2nd line, sample from 04/17/2024, 1.325 mg/L. As can be seen from the results, the HS content was in the range of 1.3 - 1.8 mg/L and contributes to the quality of irrigation water.

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PP4.4

Biogas from vegetal wastes - experimental study at laboratory scale

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Generally, the biogas is known as a gas containing methane and this can be burned as a fuel. The biogas was produced by waste of plants and animals which are decomposing, the biogas has been used on a small scale for heating, cooking and lighting in low-tech environments around the world for centuries.[1]

The study aimed to obtain biogas at laboratory scale, using biodegradable waste in order to reduce pollution and valorize it. The biogas production was carried out through anaerobic digestion, in sealed containers (400 mL), using different mixtures of plant residues, cow dung and water, respectively activated sludge for some of the experiments, taking into account the compliance with the C/N ratio between 15-25 and the humidity to be greater than 80%.

The experimental installation was realized to use a simple design, using, accessible materials. During the experiment, resulted gas was collected in a tedlar sample bag and analyzed by GS-TCD.

The results obtained from biogas analysis by gas chromatography demonstrated that the mixture inoculated with a consortium rich in methanogenic microorganisms (activated sludge) generates a biogas containing methane (approx. 7%) within 14 days, under moderate ambient temperature conditions, compared to the mixture inoculated just with cow dung. This experiment highlights the real potential of simple biodegradable waste recovery technologies in producing a renewable energy source, with a positive impact on the environment.

References

1. M. K. Jameel *et al.*, “Biogas: Production, properties, applications, economic and challenges: A review,” *Results Chem*, vol. 7, p. 101549, 2024, doi: https://doi.org/10.1016/j.rechem.2024.101549.

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PP4.5

Synthesis of TiO_2-coated fiberglass material for degradation of pharmaceutical contaminants from wastewater

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The increasing presence of persistent and non-biodegradable pharmaceutical compounds in wastewater has become a critical environmental issue due to their toxicity and potential impact on the environment and human health [1]. Among these contaminants, antibiotics such as azithromycin are of particular concern, as they contribute to the development of antimicrobial resistance and are poorly removed by conventional wastewater treatment technologies [2].

This work focused on the development and evaluation of photo-oxidative functional materials using immobilized titanium dioxide on different types of fiberglass substrates, including stratified network, fabric type, and mesh structures. The TiO_2-coated fiberglass materials were synthesized through a controlled deposition process to ensure uniform coverage and optimal photocatalytic properties. The photocatalytic performance of the obtained materials was assessed under UV irradiation using azithromycin as a target pollutant. Degradation efficiency was monitored and confirmed by the chemical oxygen demand analysis.

In this study, three functionalized materials (named 1A, 1B, and 1C) were prepared by immersing fiberglass in a solution of styrene-butadiene-styrene (SBS) elastomer type T 166 (10% SBS) in chloroform, containing 1% TiO_2 as a photocatalyst (Figure 1).

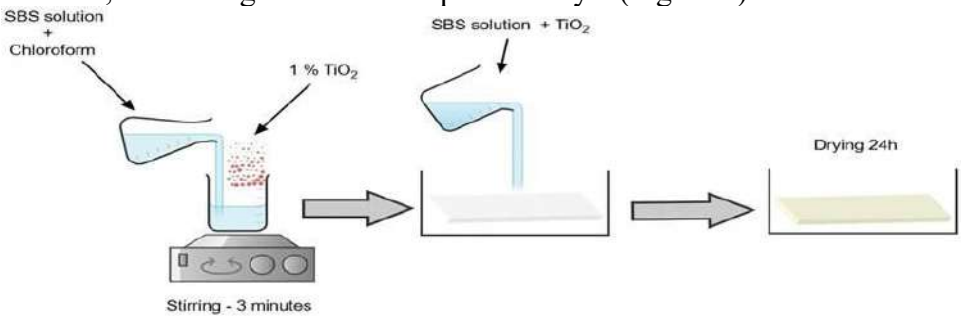

Figure 1. Schematic diagram of synthesis of TiO_2-coated fiberglass material

Although the results indicated that TiO_2 deposition was not completely uniform across the surface of the support material, but the TiO_2-functionalized fiberglass composites still showed promising photocatalytic performance. Azithromycin degradation efficiencies ranged from 60% to 77%, demonstrating the potential of these materials as cost-effective and scalable solutions for the advanced treatment of pharmaceutical-contaminated wastewater, with significant implications for environmental protection and public health.

References

1. Samrot AV, Wilson S, Sanjay Preeth RS, Prakash P, Sathiyasree M, Saigeetha S, Shobana N, Pachiyappan S, Rajesh VV, Sources of Antibiotic Contamination in Wastewater and Approaches to Their Removal - An Overview, Sustainability, 15(16):12639, 2023
2. Castro-Jiménez CC, Saldarriaga-Molina JC, García EF, Torres-Palma RA, Acelas N, Azithromycin removal from water via adsorption on drinking water sludge-derived materials: Kinetics and isotherms studies. PLoS ONE 20(1): e0316487, 2025

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PP4.6

Modified carbonaceous adsorbents for removal of sulphide and nitrite ions from water

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Activated carbons are ideal carriers for catalytic metals or are used as catalysts alone. In this work a broad spectrum of carbonaceous catalysts obtained by oxidation of activated carbons of local origin and/or impregnation with catalytic metals (Cu, Fe, Ni, Cr, Mn) were tested for removal of sulphide and nitrite ions from water. The experimental tests of sulphide and nitrite ions removal were carried out in a semi-pilot installation, equipped with an air bubbler and a container with an alkaline solution, to capture aerated SO_x and NO_x gases (Figure).

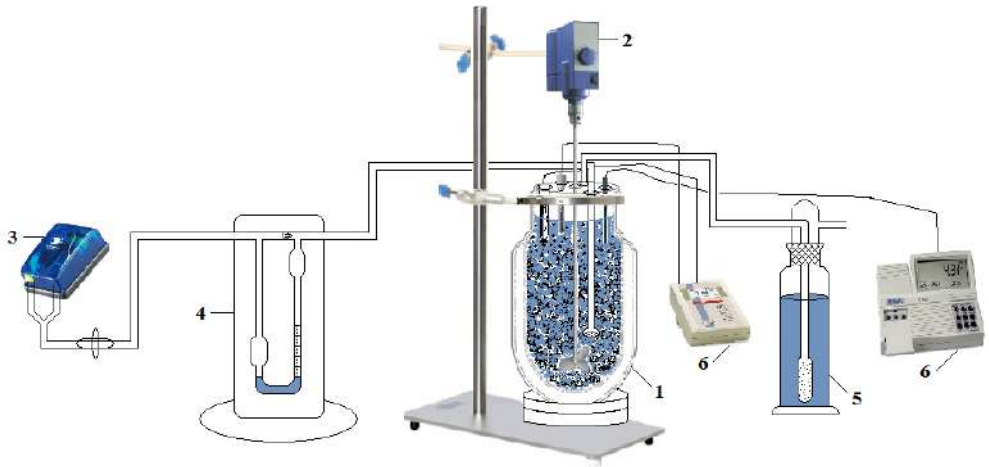

Figure. Schematic diagram of the semi-pilot installation for the removal of sulphide and nitrite ions from water. 1- Reactor; 2- stirrer; 3- air pump; 4- air meter; 5- gas capture vessel; 6- multi-parameters.

The capacity of carbonaceous catalysts for the removal/oxidation of sulphide and nitrite ions in the presence of oxygen depends on several factors: the nature of the carbonaceous support; the type of surface modification of carbonaceous support (through oxidation and impregnation with metals); the type of metal impregnated on the surface.

Comparative analysis of carbonaceous catalysts to remove sulphide ions (by adsorption and oxidation) from water highlight samples modified with nickel, manganese and copper ions (CAPrO-36Mn, CAPrO-36Ni, CAPrO-36Cu, CAPO-23Mn, CAPO-23Ni, CAPO-23Cu).

In the case of removal of nitrite ions from water (by adsorption and oxidation), the obtained results highlight samples modified with iron ions, copper oxides and manganese oxides having a removal capacity for nitrite ions of 90% (CAPrO-36Fe, CAPO-23Fe, CAPr-Mn_xO_y, CAPr-CuO).

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PP4.7

Testing of carbonaceous composites obtained by the hydrothermal method for the removal of nitrite ions from water

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Activated carbons are efficient adsorbents for the removal of inorganic species from water, including nitrite ions (NO_2^-), which are pollutants with toxic effects on health and the environment [1, 2]. The aim of this study was to evaluate the potential of activated carbons obtained via hydrothermal synthesis and fluidized-bed activation (ACCN-1, ACCN-Co1, ACCN-Mn1, ACCN-Cu1, ACCN-Ni1) for the removal of nitrite ions from water.

The testing of carbonaceous adsorbents prepared by the hydrothermal method for nitrite ions removal was conducted under static conditions, at a solid-to-liquid ratio of 1:100. After 24 hours of contact and agitation, the concentration of nitrite ions, the pH, and the conductivity of the solution were determined. Comparative analysis of nitrite ions adsorption from water highlighted the ACCN-1 samples modified with nickel and manganese. Comparative analyses of the adsorption capacity of nitrite ions from water, highlights samples modified with nickel, manganese and copper (Figure 1).

The results indicate that carbonaceous adsorbents obtained via the hydrothermal method have an efficient capacity to retain nitrite ions from water, and modification with transition metal ions significantly improves their adsorption performance. The best results were obtained for the samples impregnated with nickel and manganese. These findings demonstrate the influence of metal modification on adsorption efficiency and suggest the potential for optimizing adsorbents for the removal of inorganic species from water.

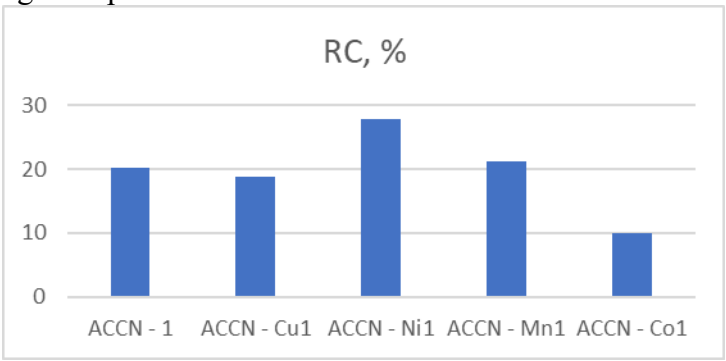

Figure 1. Removal capacity of carbonaceous composites for nitrite ions

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References

1. Gierak A, Łazarska I. Adsorption of nitrate, nitrite, and ammonium ions on carbon adsorbents. Adsorption Science & Technology 2017, 35(7-8):721-727. 10.1177/0263617417708085
2. Petrović, J.; Ercegović, M.; Simić, M.; Koprivica, M.; Dimitrijević, J.; Jovanović, A.; Janković Pantić, J. Hydrothermal Carbonization of Waste Biomass: A Review of Hydrochar Preparation and Environmental Application. *Processes* 2024, *12*, 207. https://doi.org/10.3390/pr12010207

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PP4.8

The remediation of high contaminated soil by POPs using biotechnology approach.

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Soil is an important and non-renewable natural resource which is an essential component of agriculture production with the capability of supporting the ecosystems on which economic activities and livings rely. The contamination of soil by toxic substances is an important issue worldwide. The aim of the article is to test of environmentally friendly approach for the remediation of intensive POPs contaminated soil in laboratory conditions. The following objectives were realized for this purpose: the study of one high contaminated site by POPs substances for the environmental risk assessment procedure; and the laboratory experiment for the remediation high contaminated soil using biotechnology approach. The selected POPs contaminated site was studied in detail for the soil and geological condition, POPs concentration and spectrum, which included sampling, laboratory analysis, determination of hotspots and contamination area, evaluation of the contaminated soils volume, the conceptual model elaboration for the risk assessment, and recommendation for the selection of the appropriate remediation technology. A specific project design includes several steps: project planning; construction and startup of bioremediation system; project operation, maintenance, and monitoring of the remediation process. A bench scale laboratory experiment was carried out for soil remediation which included the following steps: the determination of the contamination level, the analysis of the nature and the potential of existing microbial populations, and the evaluation of the effect of various additives on remediation. The fertilizer supplement was prepared from the local materials for the acceleration of the bioremediation process as follows: 40 % of iron powder (0.3 – 0.50 mm); 50 % of small wood shavings; 10 % of composted chicken manure. This fertilizer was used as an additive to the soil in the amount of 5 and 10% of the soil mass. The soil treatment after the fertilizer addition included cycles of anaerobic and aerobic conditions like "DARAMEND" technology. The anaerobic condition phase included soil hydration up to 70% of the maximum molecular moisture capacity, heating to 30^0 C and isolating from the air. This phase lasted for 14 days. The aerobic condition phase included the open-air condition for the temperature 20 – 25^0 C, soil loosening and drying up to 20% of the humidity. This phase lasted for 7 days. Two series of remediation had 8 cycles; two series had 4 cycles. One blank series was realized too. Every series was made in three repetitions. The total number of the functional groups of microorganisms, which are involved in nitrogen transformation processes, was determined by the experiment. After the experiment the initial soil pollution of POPs 500 – 650 mg/kg was decreased up to 70 – 85 % from initial contamination. The total number of microorganisms also was increased in the interval 40 – 120 % compared to the blank experiment. The results showed a significant reduction of POPs in soil due to changes in redox potential and increased microbial activity, which drives POPs degradation and detoxification. The concentration of toxic substances decreased from 600 – 700 mg/kg to 100 – 150 mg/kg. The principal conclusion is that the bioremediation technologies are perspective, cost-effective and simple approach among all methods for the remediation of contaminated soils.

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PP4.9

Chemical composition and pollution level of the Dniester river in the section town of Dubăsari – town of Vadul lui Vodă. Period 2020-2024

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The Republic of Moldova is a country poor in water resources, including surface water. Among the most important flowing water courses are the Dniester River and the Prut River. The Dniester River basin occupies about 57% of the country's surface and its waters are used as a source of drinking water, economy, energy, irrigation and recreation for over a million people. One of the consequences of river water consumption is an advanced level of anthropogenic pollution. The main sources of pollution of the Dniester waters are represented by domestic water from urban and rural settlements, waste water from industrial and agro-food enterprises, runoff from livestock complexes, runoff from irrigated lands, drained waters and others. One of the causes of the deterioration of water quality is also the advanced degree of pollution of the river's tributaries. In the section of the Dniester from the town of Dubasari to the town of Vadul lui Voda. Two tributaries flow into it – Raut and Ichel, which contribute to the increase in the pollution level of the main river. In order to assess the chemical composition of the Dniester waters in the given section and to estimate the influence of the tributaries on the quality of the Dniester waters, water monitoring data were analyzed, carried out by the research team in the period 2020-2024. Water samples were taken from the Dniester, upstream and downstream of the discharge of the Raut and Ichel tributaries, as well as from their mouths.

The results of the monitoring of the Dniester River in the expected portion in the period 2020-2022 show the following. Due to the processes taking place in the Dubasari reservoir, the Dniester waters downstream of it are characterized by a changed composition, compared to the upper Dniester portion. This chemical composition of the waters is additionally modified due to the ingress of waters from the right tributaries, the main effect of which is the Raut River.
The pronounced influence of the Raut on the content of the main ions and mineralization of the Dniester waters has been demonstrated. This tributary contributes to the increase in the total hardness and mineralization of the river waters. Similarly, downstream of the discharge into the Dniester of the Raut River, a decrease in the share of calcium and hydrogen carbonate ions and an increase in the share of magnesium, sodium, potassium and sulfate ions are observed.

The oxygen regime of the river during the period under review was generally within the norm. According to this parameter, waters can be characterized as pure or moderately polluted. Hardly degradable dissolved organic substances were detected in quantities that characterize waters of the III quality class – moderately polluted waters. Pollution with such substances is carried out predominantly by anthropogenic means, which indicates the pressure of human activity on the ecochemical state of the river.

The presence of mineral forms of biogenic elements denotes the recording of increased concentrations of phosphate ions, which creates premises for the development of eutrophication processes in waters, which is a negative factor for the studied ecosystem.

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PP4.9

Radon under observation: an example of participatory involvement in monitoring and remediation

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The project "Radon under Observation: an Example of Participatory Involvement in Monitoring and Remediation" aims to raise public awareness of the health risks associated with radon exposure, through the Citizen Science approach.

The Citizen Science initiative refers to the voluntary involvement of citizens in scientific research, activities, or projects, working alongside researchers to collect data, interpret results, and contribute to real-world problem-solving.

The project began in September 2024 in Arad, Romania, where 34 passive radon detectors were deployed in 21 households for a monitoring period of three months. After this period, in homes where the reference level of 300 Bq/m³ was exceeded, active radon monitoring devices (ICA) were installed to continuously record radon concentrations and environmental parameters for an additional six months.

Based on the monitoring results, one of the participating households was selected for the implementation of a passive sub-slab depressurization system, as a remediation measure to reduce indoor radon levels.

Beyond data collection, the project fosters community engagement, environmental education, and collaboration between citizens and experts in radiation protection. By combining scientific research with active public participation, it represents a practical and replicable model for local radon risk management, contributing to both public health protection and awareness.

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PP5.1

Affordable and rapid ELISA methods for determining allergens in food products

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Food allergies are a global public health problem, capable of causing serious reactions, including anaphylaxis. Most allergic reactions are caused by nine common food sources, including milk, soy, eggs, peanuts, fish, crustaceans, wheat, tree nuts and sesame. The risks associated with the presence of hidden allergens in food products have increased the need for their accurate and rapid identification.

In the Republic of Moldova, food legislation is harmonized with that of the European Union. The crucial importance of clear labeling of the 14 main allergens and mandatory information on food products, to ensure a high level of consumer protection, is established by Law no. 279/2017. At the same time, Government Decision no. 84/2024 (annex no. 2) establishes the modalities for providing information on the presence of substances that may cause allergies or intolerances in non-packaged culinary products.

Several analytical methods are used for allergen detection: Polymerase Chain Reaction (PCR), Liquid Chromatography coupled with Mass Spectrometry (LC-MS) and ELISA (Enzyme-Linked Immunosorbent Assay). Of these, ELISA is the most commonly applied in routine laboratories, due to its high sensitivity, specificity, short analysis time and affordable costs. The ELISA method works by the reaction between monoclonal antibodies and allergenic proteins, generating a colorimetric signal proportional to the concentration of the antigen. Standardized ELISA kits allow the rapid identification of various allergens in raw materials, baked goods, snacks or processed meat. This method has a number of advantages that make it particularly useful in the field of food safety.

The kits are easy to use and can be applied even by personnel with minimal training, thanks to standardized procedures and clear instructions. In addition, they provide results in a very short time, an essential aspect in the local food industry, where prompt detection of allergens can prevent the placing of contaminated products on the market. At the same time, these kits are cost-effective, offering an affordable alternative compared to other complex methods, without compromising the accuracy or reliability of the results.

The use of ELISA methods by local producers constitutes an efficient, rapid and affordable solution for the detection of food allergens. Due to their sensitivity, specificity and ease of use, they play a crucial role in ensuring food safety, protecting public health and supporting compliance with regulations in force in the Republic of Moldova.

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PP5.2

Microencapsulation of Jostaberry extract in combined biopolymer carrier agents

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Research has shown that most biologically active compounds (BAC) derived from plant sources are unstable in food environments. Flavonoids, including anthocyanins, vitamins, and pigments, degrade and lose their antioxidant activity (AA) at high temperatures, pH fluctuations, exposure to light and moisture, in the presence of oxygen, oxidative enzymes, *etc*. However, several studies have demonstrated that encapsulation of phytochemicals in biopolymer matrices is an emerging technique that enhances their stability, protects sensitive compounds from adverse environmental factors, and allows for the controlled release of BAC.

Previous research [1] has shown that jostaberry (*Ribes* × *nidigrolaria*) is a rich source of phytochemicals with strong AA, as demonstrated by DPPH and ABTS assays. However, after drying, jostaberries become sticky and gummy, making them difficult to grind into a powder. The incorporation of whole berries into food products affects their sensory properties due to the presence of solid particles resulting from the fruit's thick skin and seeds.

The aim of this study was to develop a method for the microencapsulation of jostaberry extract (JE) in combined biopolymer matrices, with the goal of obtaining stable microparticles for subsequent use in food formulations or supplements with enhanced biological value.

As a result, a simple method for the microencapsulation of JE was developed using combinations of biocompatible carrier agents: maltodextrin-nutriose (resistant dextrin)-pectin, and maltodextrin-nutriose-sodium alginate. The encapsulated products were freeze-dried to obtain water-soluble microparticles with a good yield (87.7% and 88.9%) and high biological value. Furthermore, the AA of the encapsulated compounds, determined by ABTS and DPPH assays, as well as the polyphenol and anthocyanin content, were practically unaffected by the lyophilization process. Analysis of the physicochemical properties and biological potential of the microparticles showed high retention efficiency of BAC in both biopolymer combinations at the time of manufacture and after 12 months of storage. Microstructure analysis by scanning electron microscope revealed that the microparticles had varied sizes (up to 0.1 mm) and irregular shapes, some surfaces appeared rough and porous, as a result of the sublimation of ice crystals during the lyophilization process. The freeze-dried microparticles, regardless of their structural characteristics, maintained stable AA, color, and non-adhesive properties throughout the storage period under ambient, dark conditions.

Based on the results obtained, it can be concluded that the developed encapsulation technique is suitable for the formulation of functional foods and dietary supplements, offering potential health benefits to consumers.

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References

1. Bulgaru, V.; Gurev, A.; Baerle, A.; Dragancea, V.; Balan, G.; Cojocari, D.; Sturza, R.; Soran, M.-L.; Ghendov-Mosanu, A. Phytochemical, Antimicrobial, and Antioxidant Activity of Different Extracts from Frozen, Freeze-Dried, and Oven-Dried Jostaberries Grown in Moldova. Antioxidants 2024, 13, 890. https://doi.org/10.3390/

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PP5.3

Antioxidant activity assessed through simulated *in vitro* digestion of high-protein raw materials

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Plant-based proteins provide a sustainable, cost-effective, and health-conscious alternative to animal proteins. They can be consumed directly as protein sources or incorporated into various food products to enhance amino acid profiles and improve overall nutritional value. Thanks to their rich nutrient content and affordability, plant-based protein sources have emerged as an attractive and innovative resource in the modern food industry.

The research aimed to investigate the impact of *in vitro* gastrointestinal digestion on the antioxidant activity (AA) of different plant raw materials: chickpea flour (CPF), hazelnut cake (HOC), pea protein isolate (PPI), soy protein concentrate (SPC) and soy protein isolate (SPI). The study considered their protein content, amino acid profiles, as well as the levels of mineral salts and polyphenols. Thus, the main objective was to evaluate how simulated digestion influences the potential of biologically active compounds present in plant protein sources.

The in vitro digestion of the analyzed samples (hydroalcoholic extracts) was carried out according to the INFOGEST 2.0 protocol. The AA of the samples after simulated gastrointestinal digestion was assessed using the DPPH and ABTS methods.

In samples collected after simulated gastric and intestinal digestion, Trolox equivalent antioxidant capacity was determined using both the DPPH and ABTS methods. The study revealed that the samples obtained after intestinal digestion exhibited notable AA, with the highest value recorded for HOC (1.25 mg TE/g DW) and the lowest for CPF (0.32 mg TE/g DW) in the DPPH assay. The values obtained using the ABTS method were comparatively higher, with a maximum of 3.83 mg TE/g DW for HOC and a minimum of 0.62 mg TE/g DW for SPI.

The AA values in the DPPH test did not differ significantly for the CPF, PPI and SPI samples, ranging between 0.28 and 0.34 mg TE/g DW. In contrast, SPC showed a moderately higher activity, of 0.69 mg TE/g DW. HOC demonstrated the highest AA, of 1.25 mg TE/g DW.

In the ABTS test, the CPI and SPI samples had the lowest values, measured at 0.62 and 0.87 mg TE/g DW, respectively. PPI demonstrated a higher AA, of 2.14 mg TE/g DW. SPC and HOC had the highest antioxidant activity, measured at 3.11 and 3.83 mg TE/g DW, respectively.

The results obtained can be explained by the fact that many phenolic compounds are lost along the gastrointestinal tract and, as a result, the AA of samples after digestion decreased. The loss of polyphenols explains the lower values of AA in the DPPH assay, this free radical is quenched in particular by polyphenols through the effects of electron transfer, proton transfer, or hydrogen atom transfer. The high values of AA in the ABTS test were due to the process of hydrolysis and denaturation of plant-based proteins in the gastrointestinal tract. Protein denaturation and hydrolysis during digestion increased AA in the resulting hydrolysates due to the release of amino acids responsible for AA.

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PP5.4

The influence of long-term aging on the quality parameters of red wines stored in the Mileștii Mici underground cellar

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This study investigates the impact of long-term aging on the quality parameters of red wines stored in the Mileștii Mici underground cellar, an internationally renowned site known for its optimal preservation conditions and home to the world's largest wine collection. Three wine samples were analyzed: *Cabernet Sauvignon* vintage 1989, *Cabernet Sauvignon* vintage 2008, and *Negru de Mileștii Mici* vintage 1986.

Physicochemical parameters, including alcohol content, total and volatile acidity, total and non-reducing extract, phenolic compounds, and color intensity were assessed using OIV-recommended standard methods. Sensory evaluation was carried out by a certified panel of experts using the 100-point scoring system.

The results revealed significant differences between the samples, influenced by both grape variety and aging duration. Alcohol content ranged from 12.3% to 14.5% vol., while total acidity varied from 4.6 to 5.8 g/L as tartaric acid. Older samples exhibited higher concentrations of polyphenols and anthocyanins, indicating increased color stability and a more evolved phenolic profile. *Cabernet Sauvignon* 1989 and *Negru de Mileștii Mici* 1986 stood out with intense color, characteristic of long-aged wines.

From a sensory perspective, *Cabernet Sauvignon* 1989 and 2008 scored above the minimum threshold for PGI classification, distinguished by complex aromas of ripe red fruits, spicy notes, and well-integrated tannins. In contrast, *Negru de Mileștii Mici* 1986 received a slightly lower score, likely due to decreased freshness and aromatic intensity associated with excessive aging.

This study highlights the essential role of aging in enhancing the sensory and structural attributes of red wines. Prolonged maturation contributes to greater aromatic complexity, increased phenolic stability, and overall appreciation, confirming the oenological value of wines preserved under optimal underground cellar conditions.

However, a potential limitation of this study lies in the small number of samples analyzed. Further research on a broader range of wines from different vintages and varieties, aged under similar conditions, is recommended to validate and expand upon these findings.

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PP5.5

Characterization of phenolic compounds and chromatic properties of local red wines

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The phenolic composition of red wines plays a fundamental role in defining their sensory attributes and stability. Among these compounds, proanthocyanidins oligomers and polymers of flavan-3-ols—directly influence wine structure, astringency, color intensity, and aging potential. This study aimed to evaluate the phenolic profile, with particular emphasis on proanthocyanidin content, in two indigenous grape varieties from the Republic of Moldova: Feteasca Neagră and Rara Neagră, focusing on color indices as key quality indicators.

The wines were produced in the Microvinification Laboratory of the Oenology Department at the Technical University of Moldova. Grapes were sourced from various viticultural zones, and different winemaking techniques were applied to highlight the influence of geographical origin and technological factors on the final composition. Analytical methods included spectrophotometric measurement of color intensity and hue, the Folin–Ciocalteu assay for total phenolic content, and the Bate-Smith method for proanthocyanidin quantification.

The results showed that although wines made from the same grape variety but grown in different regions exhibited comparable physicochemical parameters, their chromatic and phenolic profiles differed significantly. Feteasca Neagră wines demonstrated higher color intensity and a greater concentration of both total phenolics and proanthocyanidins compared to Rara Neagră, whose wines displayed lighter coloration. These differences can be attributed to the intrinsic genetic potential of the varieties, as well as to terroir effects.

In conclusion, this study emphasizes the importance of phenolic compounds in shaping the identity and quality of red wines, while highlighting the oenological value of native Moldovan grape varieties. The findings confirm that Feteasca Neagră and Rara Neagră contribute significantly to the diversity and territorial expression of high-quality wines from the Republic of Moldova.

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PP5.6

Quality of confectionery products using jostaberry extract as a natural colorant

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In the context of concerns about health and food quality, there is a growing trend to prefer natural and healthy food products. This trend is also reflected in the food industry, including the production of confectionery products. Replacing artificial ingredients with natural and healthy options is becoming increasingly important for producers and consumers alike, which not only ensure an authentic taste and pleasant aroma, but can also contribute to improving the nutritional quality of these products. An ingredient with potential for use as a natural colorant in candy making is the jostaberry, which is a hybrid between black currants and gooseberries. Jostaberry is rich in vitamins, minerals, and antioxidant compounds, which can give candy superior nutritional value as well as a distinct, pleasing color.

The purpose of the work was to analyze the effect of jostaberry extract, as a natural dye, on the quality indices of candies.

The hydroalcoholic extract of Josta was obtained by mixing crushed berries with a 60% alcohol solution in a 1:2 ratio. The extraction process was assisted by ultrasound at 25 °C and 37 kHz for 20 min. The mixture was then centrifuged, and the resulting supernatant was filtered, concentrated, and stored at 4 °C until use in the candy manufacturing process. Candy samples with added jostaberry extract in concentrations ranging from 1.5% to 5% were prepared.

The results obtained showed that the sensory and physicochemical parameters were within permissible limits. The optimal scores for sensory evaluation were recorded in samples containing 3.5% and 5% jostaberry extract. In all samples, the moisture content ranged from 8.8% to 13.6%, remaining within the acceptable limit of 16% maxim for this category of candies. The acidity of the samples increased slightly with higher concentrations of added jostaberry extract. The jostaberry extract had a positive influence on the textural properties of the candy samples. As the extract concentration increased, a slight decrease was observed in hardness, cohesiveness, gumminess, and chewiness, while maintaining the texture characteristics typical of this type of confectionery products. Regarding color parameters, these changed proportionally with the addition of jostaberry extract: sample brightness decreased, while red-green and yellow-blue values indicated an intensification of red and blue hues, respectively.

The study demonstrated that jostaberry extract can be successfully used as a natural colorant in candy production, contributing not only to improving visual appeal by intensifying red and blue hues, but also to the overall quality of the products. Given its nutritional and biological potential, jostaberry extract represents a promising natural alternative to synthetic additives, supporting the development of healthier and more attractive confectionery products, in line with current consumer preferences.

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PP5.7

Non-dairy probiotic drinks based on local raw materials

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Probiotic drinks have gained popularity as a useful and popular way to improve overall health and digestive function. A review of the benefits and potential drawbacks of these fermented beverages reveals that they have many advantages that can be beneficial for health. Consuming probiotic drinks can boost immunity, improve nutritional absorption, and support good digestive health by restoring the balance of intestinal flora. In addition, they may soothe gastrointestinal problems, reduce inflammation, and decrease the risk of contracting certain infections. Probiotic drinks are also a delicious alternative to pharmaceutical preparations and are easy to incorporate into your daily routine.

The non-dairy fermented probiotic drinks were prepared based on wort, molasses with the addition of extracts rich in bioactive compounds: red grape pomace extract and sea buckthorn extract. The use of extracts rich in polyphenols and carotenoids allows for the combination of probiotic and prebiotic properties. Apple juice and artisanal bran were inoculated with strains of Lactobacillus and stored under anaerobic conditions at 37°C using a Bugbox anaerobic chamber. Samples were taken at regular time intervals and the colony forming units (CFU) of bifidobacteria and lactobacilli were counted. In addition, the dry matter content and pH were measured.

To monitor the fermentation process of the beverages, the growth rate of the number of producing microorganisms –NTG—x-I(days) was determined. In all analyzed samples, the latent adaptation phase is relatively short, the accelerated-fast phase (3-4 days). Thus, the fermentation process of the beverages can be completed in 6-10 days. S

Since the production process involves stages with colloidal phases that are unstable over time, which influence the stability and shelf life of the product, the ability of clay-based materials to clarify and stabilize the developed probiotic drinks was tested and the technological scheme for their production based on local raw materials (bran, molasses, artisanal borscht) was developed.

Keywords: probiotic drinks, prebiotics, fermentation, stabilization, clay-based materials.

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PP5.8

The susceptibility of orange wines to oxidation

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Orange-type wines, obtained by long maceration of white grapes with skins and seeds, are an increasingly popular category with consumers for their complex character, intense color and distinct tannic structure.

Monitoring the susceptibility to oxidation becomes an essential parameter in ensuring the quality of the final wine. By understanding the oxidative mechanisms specific to this type of wine and applying appropriate assessment methods, winemakers can adapt the technological process in order to maintain the balance between authenticity and stability [1].

To evaluate and manage the effects of oxidation in the reference wines, the POM-Test (Polyphenols Oxidation Measurement Measurement Test) method was applied. This allows quantification of the degree of oxidation of polyphenols and gives a clear picture of the stability of the wine in the presence of oxygen.

The study investigated Orange wines obtained from the Viorica and Rkațiteli grape varieties, demonstrating the significant influence of maceration duration on oxidation susceptibility. With the application of maceration on the berry, even for a short period of time (1-2 months), a reduction of this parameter was observed. Subsequently, starting from the third month of maceration, the values become almost negligible (0.5%, 4.0%, 3.0%,). This phenomenon can be explained by the increased extractability of phenolic compounds (mainly tannins) from skins and seeds with pronounced antioxidant properties, although during maceration oxidation of another subgroup of phenolic substances with antioxidant properties - cinnamates (C6-C3) - occurs. The color intensity (A420) reaches its maximum value after 3 months of maceration with a slight subsequent decrease. This coincides with the lowest oxidizability observed. The same is true for Rkațiteli Orange wine, except that the maximum value of color intensity (A420) and minimum oxidizability are observed after 2 months of maceration on the barrel.

From a technological point of view, these results are decisive for the optimization of the maceration time in order to obtain wines with maximum intensity, characteristic of Orange wines and maximum resistance to oxidation. These periods are specific for wines from different varieties.The optimal end points can be determined by monitoring color intensity and performing the POM test.

Key words: orange wines, grapes, oxidizability, oak maceration, phenolic compounds

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References

1. Sclifos, A., Covaci, Ec. The origin and the trend of orange wines. In: *Scientific Stydy&Research, Chemistry&Chemical Engineering, Biotechnology, Food Industri*, Volume 30, SCSCC6, 2024,. Nr 3 ISSN 1582-540X

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PP5.9

Application of a new herbal drug based on fennel seed extract for the treatment of dental diseases

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The search for promising therapeutic agents for the treatment of oral mucosal and periodontal tissue diseases remains a pressing issue in modern dentistry. Currently, various herbal drugs such as tinctures of eucalyptus and calendula, as well as drugs like Salvin-1 and Maraslavin, are used for these purposes. However, they have several disadvantages, including low efficacy, unpleasant taste, irritating effects, and low pH values (below 4.5), which contribute to significant demineralization of tooth tissues, especially in children [1, 2].

For this purpose, the herbal medicine Phenglycol was elaborated, the main component of which was an alcohol extract of fennel fruits on a glycerin base. Phenglycol was clinically tested on 500 patients (adults and children aged 6 to 50 years) in various dental clinics in Moldova, as well as in the Research Institute of Dentistry and the Central Research Medical Institutions of Moscow. Clinical trials were conducted on patients with catarrhal, hypertrophic gingivitis, periodontitis, alveolitis, pericoronitis, pharyngitis, chronic recurrent aphthous stomatitis, multiforme exudative erythema, lichen planus, ulcerative necrotic gingivostomatitis.

For the treatment of periodontal tissue diseases, Phenglycol was used in the form of applications, and it was used in the form of irrigation and rinsing for diseases of the oral cavity membrane. Clinical observations had shown that Phenglycol eliminates inflammation in the area of the mucous membrane of the gum after 3-4 sessions, eliminates their bleeding, had a deodorizing, analgesic and bactericidal effect, a pleasant smell and taste.

Treatment with the drug was well tolerated by patients, especially children, who willingly followed all the doctor's instructions. In comparison with the Bulgarian drug Maraslavin, Phenglycol didn`t have a decalcifying effect, as its pH ranged from 6.5 to 7.1. Phenglycol also had a more pronounced anti-inflammatory and wound-healing effect.

Thus the drug Phenglycol possessed anti-inflammatory, wound-healing, analgesic, and deodorizing properties. It was recommended for the treatment of parodontal tissue and oral cavity mucous membrane diseases in both adults and children.

References

1. Compoziţie pentru profilaxia şi tratamentul patologiilor parodontului: brevet MD nr. 2326 G2, Inventatori: ŞEPELI, F., CUŞNIR, A., ŞEPELI D. CIB A61K 35/78. Publ. 31.12.2003, BOPI nr. 12/03.
2. CUSNIR, A., et al. Aplicarea Fenglicolului în experimente şi studii clinice. In: *Medicina stomatologică.* 2008. nr. 2(7), p.15-17. ISSN 1857-1328.

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PP5.10

Application of thin layer chromatography for the analysis of sclareol in clary sage concrete

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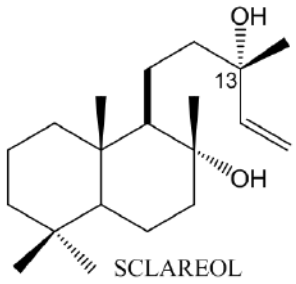
One of the main natural compounds of clary sage is sclareol, which is a valuable industrial raw material in perfumery and a component of a medicinal and essential oil plant. In the literature, there are mainly chemical methods for the quantitative determination of sclareol, but all of them are of little use for analysis in plant objects.



SCLAREOL

Thin layer chromatography (TLC) is the most convenient method for determination of individual substances in a mixture. To develop this method of analysis, the chromatographic characteristics of sclareol in the clary sage concrete were studied depending on the polarity of the solvents and their mixtures on an unfixed layer of the polar sorbent Al_2O_3, first degree of activity (layer thickness 1.8 – 2.0 mm). The results of the studies obtained were presented in Table 1.

Table 1. R_f values of sclareol and accompanying compounds of the clary sage concrete depending on the nature and composition of the mobile phase in TLC.

No.	Solvent system	*Rf* values				
		Sclareol	Components of Clary Sage Essential Oil			
		1	2	3	4	5
1	$CHCl_3$	0,08	0,24	0,37	0,56	0,75
2	Acetone – $CHCl_3$ (0,5:10)	0,41	0,55	0,70	1,0*	1,0*
3	Isopropanol – $CHCl_3$ (1:10)	0,90	0,71	1,0*	1,0*	1,0*
4	Acetonitrile – $CHCl_3$ (0,5:10)	0,46	0,64	0,74	1,0*	1,0*
5	Tetrahydrofuran – $CHCl_3$ (0,5:10)	0,12	0,35	0,49	0,62	0,78
6	Hexane – $CHCl_3$ – acetone (5:3:2)	0,42	0,65	0,78	1,0*	1,0*
7	Petroleum ether (75-85ºC) – $CHCl_3$ – acetone (5:3:2)	0,53	0,77	1,0*	1,0*	1,0*
8	Petroleum ether (64-70ºC) – $CHCl_3$ – acetone (5:4:1)	0,38	0,78	0,90	1,0*	1,0*
Note: 1.0* - the spot was on the finish line; plates (5x12 cm) with a "wet" layer of sorbent were dried (t = 65ºC) until the solvent completely evaporated; single run for solvent systems No. 1-7 and double run for No. 8.						

The optimal separation of sclareol from accompanying substances of the clary sage concrete occurred during double run in the same direction in the system of available solvents petroleum ether (64-78ºC) – $CHCl_3$ – acetone (5:4:1), the polarity of which was the lowest compared to all the studied systems. This system can be used for the quantitative analysis of sclareol by TLC in herbal extracts from clary sage [1].

References:

1. ŞEPELI D. Analiza şi standardizarea unor noi preparate medicamentoase cu aplicarea metodelor spectrale şi cromatografice / Autoreferat al tezei de doctor în ştiinţe chimice, Chişinău, 2008.

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PP5.11

Protective role of carotenoid-rich berry extracts against lipid oxidation in sunflower oil

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Oxidation is a chemical process that involves the modification of fatty acids, amino acids and vitamins, which in turn affects the organoleptic and nutritional characteristics of food. Lipids are a highly perishable fraction of food, so their storage conditions depend largely on their nature and concentration. The aim of this study was to evaluate the stabilizing effect of lipophilic extracts from sea buckthorn and rosehip fruits on sunflower oil over a period of 12 months. Physicochemical parameters (acid value (AV), peroxide value (PV), conjugated dienes (CD) and trienes (CT), p-anisidine value (PAV)) describing the oxidative states of sunflower oil and sea buckthorn and rosehip fruits lipophilic extracts during storage were analyzed.

The AV indicates the extent of the heat-induced oxidative and hydrolytic degradation of the oil and lipophilic extracts of sea buckthorn and rose hips. The AV values in the lipophilic extracts in the initial stage varied between 0.20–0.21 mg KOH/g, being higher compared to the values for sunflower oil, namely 0.17 mg KOH/g. During the storage of oil and lipophilic extracts, the AV value increased, demonstrating the accumulation of free fatty acids without exceeding the limits set by regulations. The PV determines the degree of stability of the extracts. During storage, the sea buckthorn extracts' PV increased: in sea buckthorn, the increase was within the range of 1.31 to 3.24 mmol O_2/kg; in rose hips, the range was 1.62–3.71 mmol O_2/kg; and in oil, the increase ranged from 2.82 to 5.12 mmol O_2/kg. The PV values in the lipophilic extracts are lower compared to sunflower oil due to the presence of carotenoids, i.e., antioxidants extracted from the pulp of berries, which can neutralize singlet oxygen and eliminate active free radicals involved in the lipid peroxidation process. CD and CT represent indicators with which to measure the oxidative state of oils, which are produced from unsaturated fatty acids as a result of the rearrangement of double bonds. An increase in both CD and CT was observed in all samples throughout the 12 months. Sea buckthorn extracts had the lowest levels, ranging from 7.20–10.95 µmol/g (CD) and 3.34–5.09 µmol/g (CT). Rosehip extracts ranged from 7.25–11.31 µmol/g (CD) and 3.37–5.33 µmol/g (CT), while sunflower oil exhibited values of 8.60–13.66 µmol/g (CD) and 3.99–6.35 µmol/g (CT). The PAV measures the number of secondary oxidation products, such as carbonyl compounds (aldehydes, ketones, and their derivatives) with different carbonyl chain lengths, which can negatively affect taste and odor. During storage, the smallest number of secondary oxidation products accumulated in lipophilic extracts from berries, for which PAVs ranged from 0.986 to 0.991 u.c.

Analysis of the changes in the physicochemical properties of the investigated samples during storage for 12 months at a temperature of 4 °C and in the absence of light showed that under these conditions, the carotenoids from the sea buckthorn and rose hip extracts positively influenced the oxidative stability of the extracts in relation to sunflower oil.

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PP5.12

Optimized extraction of water-soluble bioactives from Sea Buckthorn pomace using green techniques

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Sea buckthorn (*Hippophae rhamnoides* L.) pomace, a by-product of fruit processing, represents a promising raw material for the recovery of water-soluble bioactive compounds with antioxidant, anti-inflammatory, and immunomodulatory properties. Rich in ascorbic acid, polyphenols, flavonoids, organic acids, and soluble sugars, sea buckthorn aqueous-alcoholic extracts are increasingly incorporated into functional food formulations. These extracts integrate easily into the food matrix, enhancing nutritional value and oxidative stability without significantly altering texture, while also contributing to sensory enrichment [1, 2].

This study aimed to optimize extraction conditions for obtaining high-quality water-soluble extracts from sea buckthorn pomace using eco-friendly, intensified extraction methods — namely, ultrasound-assisted extraction (UAE, 37 kHz) and microwave-assisted extraction (MAE, 180 W). A range of aqueous ethanol solvent systems (15–85% v/v ethanol) were tested at a constant temperature of 20 °C, with varying extraction times (5–35 minutes) and five different solvent ratios: 30:70, 25:75, 15:85, 20:80, and 60:40 (water:ethanol).

The optimal extraction yield (8.5% total solids and 11.2 °Brix of soluble solids) was achieved under microwave-assisted extraction for 5.5 minutes with a 60:40 water–ethanol mixture. Furthermore, titratable acidity reached 1.32 g citric acid/100 mL under MAE conditions, surpassing that of UAE (1.18 g/100 mL). Spectrophotometric analyses confirmed high levels of polyphenolic compounds, especially flavonoids and hydroxycinnamic acids, substantiating the strong antioxidant capacity of the extracts.

The results demonstrate that sea buckthorn pomace is a valuable and sustainable source of water-soluble bioactives. The use of green extraction technologies such as UAE and MAE enables the efficient recovery of these compounds while aligning with sustainable food production goals. The resulting extracts can serve as potent functional ingredients, enhancing both the health-promoting properties and market value of food products.

Keywords: bioactive compounds, extraction efficiency, fruit waste valorization, microwave treatment, natural antioxidants, polyphenol recovery, solvent systems, sustainable processing, thermal degradation, ultrasound-assisted extraction

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References

1. TACHIE, C., NWACHUKWU, I.D., ARYEE, A.N. Trends and innovations in the formulation of plant-based foods. In: Food Production, Processes and Nutrition, 2023, 5, 16. https://doi.org/10.1186/s43014-023-00129-0
2. MARCINIAK, B.; KONTEK, R.; ŻUCHOWSKI, J.; STOCHMAL, A. Novel bioactive properties of low-polarity fractions from sea-buckthorn extracts (Elaeagnus rhamnoides (L.) A. Nelson) – (in vitro). In: Biomedicine and Pharmacotherapy, 2021, 135, 111141. https://doi.org/10.1016/j.biopha.2020.111141

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PP5.13

Sensory improvement of low-fat cheesecake using β-glucans from Merlot wine yeast

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β-Glucan is a highly hydrophilic, non-starch polysaccharide noted for its capacity to modify key functional parameters of food systems, such as rheology, viscosity, texture, and sensory attributes. Its abundance of hydroxyl groups enables extensive hydrogen bonding with water molecules, thereby imparting significant water-holding capacity and gel-forming ability. Additionally, modifications through enzymatic, chemical, mechanical, or thermal treatments can tailor β-glucan's molecular structure - altering its conformation, molecular weight, and branching - to achieve targeted morpho-rheological and bio-functional properties [1]. Extensive scientific studies have highlighted the positive health impacts of β-glucans, indicating their potential in supporting immune function, regulating blood glucose levels, maintaining healthy cholesterol, and contributing to liver protection, wound healing, weight control, and lowering LDL cholesterol. In this study, the goal was to create a low-calorie dessert that not only meets nutritional benefits but also maintains favorable sensory attributes. The β-glucan used was extracted from residual yeast left after the vinification process of Merlot dry red wine, produced by the "Cricova" SA winery [2]. To develop the recipe, a chocolate cheesecake was selected, as it could mask the slight colour changes caused by the addition of beta-glucan derived from red wine yeast [3]. The preparation method involved cold processing to maximize the retention of the ingredients' beneficial properties and to monitor the rheological changes in the dessert depending on the beta-glucan concentration. To assess the effect of β-glucans on the final product, five sample variants were developed with different polysaccharide concentrations (0%, 0.4%, 0.6%, 0.8%, and 1%). Beta-glucans were combined with gelatin and water, preheated in a steam bath. Sensory analysis was conducted to evaluate the product's attributes. Among all the variants, the sample enriched with 0.6% β-glucan received the highest sensory scores, indicating optimal performance in key attributes such as visual appeal, texture, flavour, aroma, and overall acceptability.

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References

1. Trohina, A., Chirsanova, A., Boiștean, A. Rheological characteristics of beta-glucans obtained from wine lees of wines from local grapes varieties. In: The Biotechnologies, Present and Perspectives: intern. conf., 15 Dec. 2023, Suceava, Romania, 9 ed.: abstracts, Suceava, 2023, p. 21. ISSN 2068–0819. http://repository.utm.md/handle/5014/27183
2. Boiștean, A., Chirsanova, C. A., & Chioru, A. (2024). Producerea de β-glucan din drojdiile vinurilor locale produse cu utilizarea diferitor tehnologii. In: Conferința Științifică Națională "Inovația: Factor Al Dezvoltării Social-Economice", Cahul, Republica Moldova, Ediția a IX- a, 12 Decembrie, 2024. Universitatea de Stat "Bogdan Petriceicu Hasdeu" din Cahul. Cahul: Print-Caro, 2024, pp. 45-46. ISBN 978-9975-88-128-9. https://repository.utm.md/handle/5014/31857
3. Chioru, A., Chirsanova, C. A., Zacuțelu, M., & Boiștean, A. Physico-chemical and sensory changes in bread fortified with red wine. In: Modern Technologies in the Food Industry, 17-18 octombrie 2024, Chișinău. Chișinău, Republica Moldova: „Tehnica-UTM", 2024, p. 79. ISBN (pdf) 978-9975-64-472-3.

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PP5.14

Extraction of liposoluble bioactive compounds from Sea Buckthorn pomace: Optimization and antioxidant evaluation

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The sea buckthorn pomace, obtained as a by-product following juice extraction from the fruits of sea buckthorn *(Hippophae rhamnoides L.*), was subjected to drying and fine grinding processes. The resulting material was then used for the extraction of bioactive compounds using ultrasound-assisted extraction, with solvents of different types and concentrations. The aim of this study was to valorize the by-product by optimizing the extraction of bioactive compounds using non-conventional methods, in order to increase the extraction yield.

The extraction of bioactive compounds (BAC) from the vegetal matrix was carried out using ultrasound-assisted extraction, with food-grade solvents consisting of hydroalcoholic mixtures combined with refined sunflower oil, in varying concentrations: 35/65; 40/60; 45/55; 50/50; and 65/35. The extraction conditions were: a temperature of 20 ^{0}C, extraction times of 366, 372, 378, 384, and 390 seconds, and a frequency of 37 kHz. The resulting extract was centrifuged for 10 minutes at 8000 rpm, then subjected to rotary evaporation until the complete removal of alcohol, yielding an oily concentrate. The obtained extracts were characterized in terms of total bioactive compound content, particularly lutein, zeaxanthin, and Z-lutein diPalmitate, using high-performance liquid chromatography (HPLC), as well as their antioxidant activity. The results showed that using a hydroalcoholic mixture and refined sunflower oil in a 40:60 ratio, combined with an extraction time of 372 seconds, led to the highest BAC extraction yield of 72.38 mg/g. Of this amount, lutein accounted for 1.69 mg/g, zeaxanthin for 4.32 mg/g, and Z-lutein diPalmitate for 12.9 mg/g. These compounds possess the ability to scavenge free radicals, giving them significant antioxidant properties. The total polyphenol content (TPC), determined using the Folin–Ciocalteu method, reached a maximum value of 46.08 mg GAE/L in the sample with a 45/55 ratio and an extraction time of 378 seconds. This indicates that this proportion optimizes the extraction of polyphenolic compounds and highlights the significant influence of both the composition of the extraction system and the duration of ultrasonication on the efficiency of the process. The antioxidant capacity of the oily concentrate, determined using the ABTS and DPPH methods, varied depending on the solvent mixture ratio used in the extraction. The sample with a 40/60 ratio recorded the highest value using the ABTS method (0.18 mg TE/mL), followed by the 35/65 sample (0.16 mg TE/mL). In contrast, for the DPPH method, the highest values were obtained for the samples with ratios of 45/55 (39.54 mg TE/mL) and 40/60 (31.35 mg TE/mL), highlighting significant differences in the sensitivity of the two methods to the composition of the extraction mixture. The concentrate obtained through the optimized extraction of bioactive compounds from white sea buckthorn pomace is characterized by high antioxidant activity and has broad applicability in the food industry for the development of functional products with antioxidant effects. The use of this concentrate contributes to the sustainable valorization of the by-product and to the improvement of the nutritional profile of food products.

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PP5.15

Phytochemical characterization and functional development of an antioxidant digestive shot based on *Salvia officinalis* L.

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This study explores the antioxidant potential and phytochemical profile of *Salvia officinalis* L. cultivated in two regions of the Republic of Moldova—Căușeni and Nisporeni—with the goal of developing a functional digestive shot enriched with bioactive compounds. Comprehensive analyses of hydroalcoholic and lipidic extracts were performed to determine the content of polyphenols, flavonoids, and tannins, as well as antioxidant activity via DPPH assay. *UV-Vis* spectroscopy revealed absorption maxima around 670 nm, indicating the presence of chlorophylls, and at 325–400 nm, confirming polyphenolic compounds. Comparative quantification showed slightly higher concentrations of polyphenols (2.576±0.12 mg GAE/g), flavonoids (0.256±0.04 mg QE/g), and antioxidant capacity in Căușeni samples versus Nisporeni.

Building upon these findings, a novel liquid formulation was developed—a cold-processed, antioxidant-rich digestive shot composed of sage powder (15%), lemon juice (20%), fresh ginger juice (10%), natural honey (15%), spirulina (0.2%), and filtered water to 100%. The synergistic combination was designed to enhance digestive and antioxidant effects while maintaining a pleasant sensory profile. Sensory evaluation by a trained panel (n=20) revealed high acceptability scores for appearance (5/5), color (5/5), aroma (4.5/5), taste (4.5/5), and consistency (5/5), with a mean overall score of 23/25.

The product was packaged in 30–50 mL amber glass vials to ensure stability, prolong shelf life, and preserve bioactive compounds. The final formulation stands out through its potent antioxidant activity, largely attributed to the rich polyphenolic content of *Salvia officinalis* and its synergistic combination with other antioxidant-rich ingredients such as lemon, ginger, and spirulina. This antioxidant synergy helps neutralize free radicals, reduce oxidative stress, and protect cellular integrity—benefits that are highly relevant for modern consumers exposed to daily environmental and metabolic stressors. The developed shot exhibits a multifunctional profile, combining antioxidant, anti-inflammatory, antimicrobial, and digestive-stimulating properties. As a concentrated plant-based supplement, it offers a practical and natural solution to enhance the body's antioxidant defense system, contributing to overall health and preventive nutrition.

Keywords: *Salvia officinalis*, antioxidant activity, polyphenols, *UV-Vis* spectroscopy, functional food, digestive shot, DPPH assay, chlorophyll, consumer acceptability.

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PP5.16

Development and evaluation of wheat flour substitutes with hemp (*Cannabis sativa* l.) cake and inflorescence in functional noodles

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The growing demand for nutritionally enhanced foods has led to innovative formulations in staple products such as noodles. This study investigated the partial replacement of wheat flour with hemp (*Cannabis sativa* L.) by-products—specifically hemp seed cake and hemp inflorescence flour—in fresh pasta recipes, with the aim of improving nutritional composition, particularly fiber, protein, and antioxidant content.

Noodles were formulated with increasing substitution levels (5% to 30%) of either hemp seed cake or hemp inflorescence flour. Standard physicochemical analyses were conducted to evaluate acidity, dry matter, moisture content, total polyphenol concentration, and antioxidant activity using the DPPH radical scavenging assay. In addition, color parameters (*L, a, b*, ΔE, and whiteness index) were assessed to determine visual changes caused by the substitution.

The inclusion of hemp seed cake significantly increased the polyphenol content from 110.45±1.15 to 256.51±1.34 mg GAE/kg and enhanced antioxidant activity from 8.0% to 19.1%, with a strong upward trend proportional to the substitution level. Similar results were observed for samples containing hemp inflorescence, where total polyphenols increased to 249.11±1.28 mg GAE/kg and DPPH antioxidant activity reached 18.2% in the 30% replacement sample.

These results demonstrate the considerable antioxidant potential of both hemp derivatives, confirming their role as functional ingredients in pasta products. The increased antioxidant activity is closely associated with the high levels of bioactive compounds—namely polyphenols, flavonoids, and chlorophyll—naturally present in hemp by-products. The functional enrichment was achieved while maintaining acceptable technological parameters, including acidity levels within legal limits and stable moisture content.

Color analysis revealed a darker, greenish hue in hemp-enriched noodles, attributed to Maillard reactions and the presence of chlorophyll. Although color intensity increased, this change is consistent with consumer expectations for high-fiber or plant-enriched functional foods. In conclusion, the substitution of wheat flour with hemp cake or inflorescence flour represents a promising approach to developing antioxidant-rich, functional pasta. This innovation not only adds nutritional value but also supports sustainability and the valorization of agro-industrial hemp by-products in the food sector.

Keywords: hemp seed cake, hemp inflorescence, *Cannabis sativa* L., antioxidant activity, polyphenols, functional noodles, DPPH assay, wheat flour replacement.

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PP5.17

Investigation of the immunostimulatory potential of novel triazole-based preparative forms on tomato seeds under *Fusarium spp.*-infected soil conditions

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This study explores the immunostimulatory and growth-promoting properties of newly synthesised triazole derivatives used as seed treatment formulations for tomato plants germinated in soil contaminated with *Fusarium spp.* A series of 31 triazole-based compounds were synthesised and tested at concentrations of 0.1%, 0.01%, and 0.0002%, including combinations with chitosan to assess potential synergistic effects.

As biological material, tomato plants of the Brutus cultivar (originating from the Czech Republic) were used. Seeds (lot no. 271-01, Diolsem®, Republic of Moldova, 2024) were treated with the tested solutions for 8 hours. For each treatment, 20 seeds were used, and experiments were conducted in triplicate. The seeds were divided into two experimental groups. Group I seeds were germinated in sterile Petri dishes on UV-irradiated filter paper, with distilled water-treated seeds serving as control. Group II seeds were planted in soil collected from the experimental fields of the Institute of Genetics, Physiology and Plant Protection, known to be infected with *Fusarium spp.* (confirmed by molecular testing). Controls for this group included distilled water (Control I), Fitosporin (Control II), and Topaz (Control III). All plants were cultivated in a Hydro Shoot 150 growth chamber (Secret Jardin®, Belgium) under controlled conditions: 16/8 h day/night cycle, 24°C, 5000 lm/m² light intensity, and 60–65% humidity. The growth period lasted 14 days. At the end of cultivation, root and stem lengths were measured for all plants.

Biological assays revealed that most tested compounds stimulated root growth in tomato plants grown in *Fusarium*-infected soil compared to the water control. Notably, a formulation containing 0.0002% of a chromenol-triazole derivative exhibited the strongest immunostimulatory effect, with root length reaching 290 mm, while most formulations ranged from 60–90 mm and did not exceed 100–113 mm. Several formulations based on diluted hydrolysed chitosan significantly enhanced root development under infection stress. One formulation containing 0.01% of active compound in chitosan solution produced an average root length of 193 mm—substantially higher than both the water control (24.83 mm) and chitosan alone (115 mm), suggesting a synergistic immunostimulatory effect. Similar effects were observed for six other 0.01% formulations, with root lengths ranging from 160 to 178 mm.

These results demonstrate the promising potential of triazole-based compounds, particularly in combination with chitosan, as effective immunostimulatory agents for enhancing plant resilience against *Fusarium* infection. Their application in seed treatment could represent a valuable strategy for integrated crop protection.

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PP5.18

Valorization of unfermented red grape pomace: *Cabernet Sauvignon* and *Rara Neagră* in the Ccntext of circular economy

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Grape pomace is an agro-industrial by-product of significant added value due to its high content of biologically active compounds, including polyphenols, dietary fibers, oligosaccharides, proteins, fatty acids, vitamins, and minerals. In this context, the present study aimed to obtain and characterize hydroalcoholic extracts from unfermented pomace derived from the red grape varieties *Cabernet Sauvignon* and *Rara Neagră* (2024 harvest), processed under micro-winery conditions at FTA/UTM.

Through a rigorous experimental approach, optimal conditions for the extraction of bioactive compounds were determined. The evolution of physicochemical and chromatic parameters was monitored during the process, while total polyphenol and anthocyanin contents, along with antioxidant capacity, were quantified. UV-Vis absorbance spectra recorded within the 400–700 nm range confirmed the presence and intensity of specific phenolic compounds. The results indicated that citric acid acidified extracts from *Rara Neagră*, at extraction temperatures of 55°C and 40°C, exhibited maximal absorbance values, reflecting a high phenolic content and enhanced anthocyanin stability under acidic conditions. Total phenolic content ranged from 15.22 to 17.21 mg GAE/g extract for *Cabernet Sauvignon*, and from 19.04 to 28.02 mg GAE/g for *Rara Neagră*, while the antioxidant activity exceeded 85%. The dry matter content, expressed as a percentage, ranged from 24.90% to 28.00% in the Cabernet Sauvignon pomace extracts, and from 26.10% to 29.50% in those derived from *Rara Neagră*.

These findings highlight the promising potential of grape pomace extracts to be employed as functional ingredients in the food, pharmaceutical, and nutraceutical industries. Advancements in the valorization of grape pomace, viewed through the lens of the circular economy, enable a transition from agro-industrial waste management to health promotion through functional, value-added ingredients.

Keywords: wine by-products industry, pomace extracts, anthocyanin pigments, phenolic compounds.

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PP5.19

Alfalfa protein concentrate - functional ingredient for the food industry

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Animal-based foods are a major source of protein in today's diet. However, excessive consumption of red and processed meats has been associated with cardiovascular disease, diabetes, and cancer. As global concerns about environmental impacts continue to grow, it is important to note that livestock farming uses 70% of agricultural land and contributes significantly to greenhouse gas emissions. To meet nutritional needs, it is necessary to enrich traditional foods with plant-based proteins and biologically active compounds. This approach allows for the partial replacement of carbohydrates in the diet with proteins and essential amino acids. Currently, most fortified foods are based on a combination of legume and wheat proteins. The alfalfa plant (*Medicago Sativa* L.) contains proteins that represent approximately 20% of its green biomass. Its primary protein component, ribulose-1,5-bisphosphate carboxylase/oxygenase (RuBisCO), is notably richer in sulfur-containing amino acids - such as lysine, threonine, and tryptophan - compared to wheat proteins. RuBisCO accounts for approximately 75% of the total soluble protein content in alfalfa. As a non-allergenic protein, RuBisCO has been approved for human consumption as a dietary supplement since 2009, with a recommended daily intake of up to 10 g. Its wide range of reported health benefits includes anticancer, anti-inflammatory, cholesterol-lowering, diuretic, kidney stone-preventive, hypoglycemic, and immunomodulatory effects, as well as the ability to alleviate menopausal symptoms, reduce oxidative stress, and lower blood pressure. In addition to its nutritional value, alfalfa protein concentrate exhibits several functional properties, including foaming capacity comparable to that of egg white proteins, good solubility at food-relevant pH levels, and gelling ability at low concentrations across a wide pH range and moderate temperatures. In this context, the identification and development of unconventional, environmentally friendly extraction methods with high efficiency - both in terms of protein yield and minimal degradation of protein quality and phytochemical bioactivity - is of critical importance. The aim of this research was to optimize the extraction conditions for obtaining high biological value alfalfa protein concentrates suitable for applications in the food industry. The extraction conditions for alfalfa protein concentrates were optimized using both conventional and unconventional methods (including ultrasound), considering variations in pH, hydromodulus, ultrasound frequency, and application time. The influence of processing conditions on the yield, sensory, physicochemical properties, and CIELab color parameters of the concentrates was investigated. Additionally, the biological value and antioxidant activity of the extracts were assessed in relation to both extraction and storage conditions. Mathematical models were developed to analyze the impact of extraction conditions on the quality and biological value of the protein concentrates. As a result, alfalfa protein concentrate with high biological value can be recommended for the development of functional foods with potential health benefits, contributing to an improved quality of life for consumers through access to innovative and sustainable food products.

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PP5.20

Butyric fraction of dairies as determined from ^{13}C-NMR data

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In contrast to ^{1}H-NMR, ^{13}C-NMR spectra display distinct resonances for individual carbon atoms due to their broader chemical shift range.

The main spectral regions corresponding to carbon resonances include: (a) carbonyl carbons (~175 ppm), (b) carbon–carbon double bonds (–C=C–, ~130 ppm), (c) glycerol backbone (~50 ppm), (d) methylene groups (~20–35 ppm), and (e) terminal methyl groups (CH_3, ~14 ppm) [1]. The characteristic resonances of the butyric moiety can be individually assigned to its four carbon atoms by comparison with the spectrum of the tributyrin (TB) standard, as illustrated in *Figure 1*.

Thus, the butyric fraction can be quantified using various mathematical approaches, by evaluating the ratio of specific resonances of the butyryl chain against the total resonances of the corresponding carbon types across all fatty acyl species.

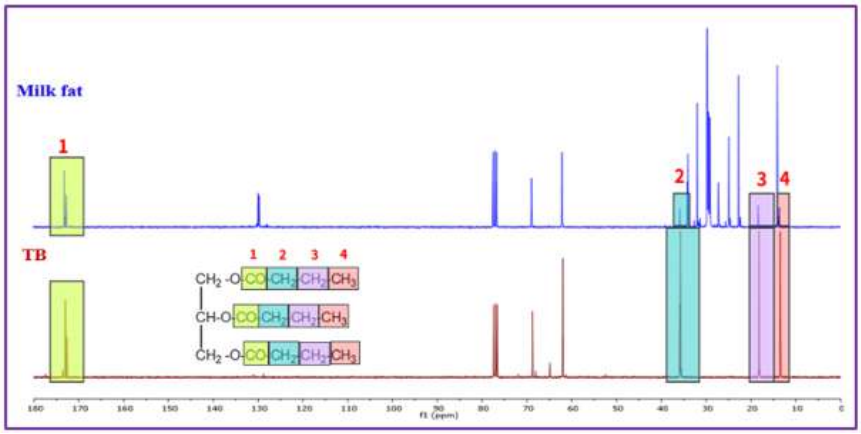

Figure 1. Stacked ^{13}C-NMR spectra of milk fat and tributyrin (TB)

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References

1. Chira, N.A., Nicolescu, A., Stan, R., Rosca, S., 2016. Fatty Acid Composition of Vegetable Oils Determined from ^{13}C-NMR Spectra. Revista de Chimie, 67(7):1257-1263.

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PP5.21

Spectral characterization of the volatile fatty acids in dairy products: ^{1}H-, ^{13}C- and 2D experiments

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Volatile fatty acids (VFAs) play a key role in the flavor and aroma profile of dairy products, especially in aged cheeses and fermented milk. These compounds, including acetic, propionic, butyric, and caproic acids, are produced primarily through microbial fermentation of lactose and lipolysis of milk fat. The presence and concentration of VFAs can be used as indicators of ripening stage, quality, and in some cases, spoilage or adulteration. Particularly, butyric acid is a marker of lipolytic activity and contributes to the characteristic sharp, pungent notes found in certain cheeses. Analytical techniques such as gas chromatography are commonly used to identify and quantify VFAs in dairy matrices.

VFA can be globally assessed through the Reichert-Meissl and Polenske value [1]. Although ^{1}H-NMR spectroscopy has limitations in determining the short chain fatty acids due to signal overlapping, ^{13}C-NMR spectroscopy, combined with advanced experiments (such as DEPT 135 and 2D experiments) may allow for the determination of the butyrate and caproate moiety in dairy foods. Preliminary experiments were conducted on both standard compounds – tributyrin (TB), methyl hexanoate (MH), methyl octanoate (MO) and methyl decanoate (MD) and on dairy fats added with standard compounds.

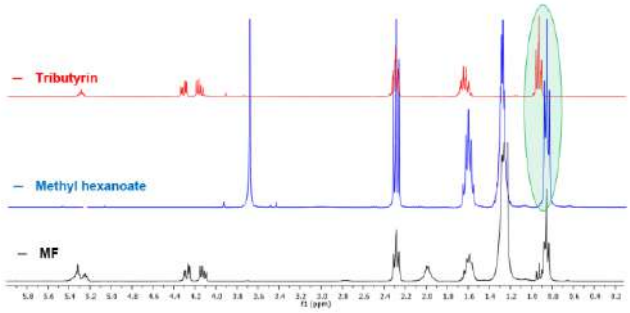

Figure 1. Stacked ^{1}H-NMR spectra of milk fat, methyl hexanoate and tributyrin

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References:

1. Bharwade, M., Balakrishnan, S., Chaudhary, N., Jain, A.K., 2017. Fatty Acid Profile and Physico-Chemical Characteristics of Milk Lipids of Kankrej Cow. Int. J. Curr. Microbiol. App. Sci., 6(8):3035-3047.

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PP5.22

Influence of rice type and boiling duration on glycemic index: Implications for glycemic control and personalized dietary recommendations

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Glycemic index (GI) management is a key component of nutritional strategies for the prevention and control of diabetes mellitus. Rice, a staple food for over four billion people worldwide, exhibits substantial variability in GI depending on its starch composition (amylose–amylopectin ratio) and cooking method. This study investigated the effect of rice type and boiling duration on GI, using the standardized ISO 26642:2010 method in a group of 10 healthy adults (aged 20–35 years, BMI 18.5–24.9 kg/m²).

Four rice types were tested: white round-grain rice (WRGR), parboiled white medium-grain rice (PWMGR), white long-grain rice (WLGR), and whole-grain long-grain rice (WGLGR). Each type was prepared using standard boiling (as per manufacturer instructions) and extended boiling (+10 minutes). Portions were standardized to provide 50 g of available carbohydrates, and capillary blood glucose was measured over 120 minutes postprandially.

The results showed a significant increase in GI for all rice types with prolonged boiling, linked to enhanced starch gelatinization and greater enzymatic accessibility. The largest percentage increase in GI was observed for whole-grain long-grain rice (+25.4% between standard and extended boiling), although it maintained the lowest absolute GI values. White round-grain rice recorded the highest absolute GI, reaching a mean of 96.2 with extended boiling.

High-amylopectin varieties (WRGR, PWMGR) displayed higher GI values, while high-amylose, fiber-rich varieties (WGLGR) showed reduced digestibility and a more moderate glycemic rise. These findings confirm that both rice selection and control of boiling time are decisive factors in managing postprandial glycemic responses.

Study limitations include the small sample size and the inclusion of only healthy participants, which may limit the applicability of results to individuals with diabetes or other metabolic disorders. Future research should include additional rice varieties (e.g., black, red) and alternative preparation methods (e.g., steaming, baking), as well as larger, more diverse participant groups, including those at elevated metabolic risk.

In conclusion, the findings underscore the importance of simultaneously adapting rice type and preparation method within personalized dietary strategies. Moderate boiling and the preference for high-amylose varieties may support better postprandial glycemic control, potentially aiding in the prevention and management of metabolic complications. These results have clinical relevance and may inform nutritional guidelines tailored to populations in the Republic of Moldova and other regions with similar dietary patterns.

References

1. Vîrlan, A.; Coșciug, L.; Țurcanu, D.; Siminiuc, R. The Influence of Rice Types and Boiling Time on Glycemic Index: An In Vivo Evaluation Using the ISO 2010 Method. In: Foods, 14, 12, 2025. https://doi.org/10.3390/foods14010012
2. Siminiuc, R.; Țurcanu, D.; Siminiuc, S. Healthy Food Basket: Sustainable and Culturally Adaptive Nutrition for Moldova. Sustainability 2025, 17, 4294. https://doi.org/10.3390/su17104294

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PP5.23

Spectral fingerprint of traditional Romanian dry cured salami – case study of *Poiana Marului Salami*

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The competitiveness of a local region, in the global markets, depends on its ability to capitalize its own areal specificities. According to this, in the food industry sector, products that are traditionally and strongly influenced by their region of origin have an important role, being certainly different from their contemporary counterparts due to their historical, cultural and social features. In this context, the place of production combined with local production knowledge, often passed down through generation, creates unique tastes which cannot be reproduced, considering this aspect as an attribute of superior quality [1,2].

Thus, it can be said that geographical indication can become a tool for promoting traditions, can increase sales by bringing value and wealth to producing localities, but can also provide satisfaction and pride to producers due to the appreciation of their lifestyle [1].

Based on the food market expansion the European Union (EU) has initiated quality programs and schemes as a legal tool for ensuring, supervising, controlling and protecting food products. Through a quality scheme, EU intends to offer equal benefits to both consumers and producers in all associated states [2]. Finding a right balance between the traditional methods and today's technology represents a real challenge for preserving natural resources and historical heritage [3].

In the frame of the European market, preserving traditional high quality local products represents an important concern. EU food quality schemes help the consumers to identify high-quality products beyond the language barriers. Preserving the quality recipe and protecting the recognized food products against fraud needs permanent attention from food researchers [4].

The main objective of this study is to establish the spectral fingerprint of Poiana Marului Salami, which is a dry cured product holding a PGI label throughout EU food quality schemes. The fingerprinting procedure aims to establish which are the main spectral characteristics which clearly differentiate this particular product from similar products of its class.

In this endeavor the FT-IR and 1H-NMR methods are used separately or in combination with chemometric methods in order to distinguish the main spectral characteristic of Poiana Marului Salami which makes it unique.

References

1. R. Crescenzia, F. De Filippis, M.G.C. Vaquero-Piñeiro, Geographical Indications and local development: the strength of territorial embeddedness. The Journal of the Regional Studies Association 2022, 56(3), 381–393;
2. C. Chifor, I.D. Arion, V.I. Isarie, F.H. Arion, A Systematic Literature Review on European Food Quality Schemes in Romania, Sustainability 2022, 14(23), 16176;
3. M. Guareschi, M.C. Mancini, F. Arfini, Geographical Indications, public goods and sustainable development goals: A methodological proposal, Journal of Rural Studies 2023, 103, 103122;
4. M.C. Todasca, M. Tociu, F.A. Manolache, 1H-NMR Spectroscopy a Useful Tool for the Sibiu Salami Geographical Indication Protection, Revue Roumaine de Chimie 2022, 67(3), 151–158.

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PP5.24

The effect of a Seaweed-based biostimulant on vitamin synthesis in *Momordica Charantia*

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Momordica charantia is a tropical and subtropical climbing plant belonging to the *Cucurbitaceae* family. Popularly known as bitter gourd, this plant is widely cultivated in South America, Asia and East Africa [1]. *Momordica charantia* contains a wide range of biologically active compounds, including proteins, vitamins, alkaloids, saponins, flavonoids, triterpenes and amino acids, due to which the plant possesses antiviral, antifungal, antibacterial, antiparasitic, antitumor and hypoglycemic properties, being considered as "green insulin" [2][3].

Vitamins are a group of organic compounds essential for the physiological functions of the body [4]. Vitamin A plays an important role in the immune system, in maintaining vision and the integrity of the skin. Vitamin C is a powerful antioxidant with a role in cellular protection against oxidative stress [5].

Seaweed-based biostimulants are natural compounds rich in phytohormones, polysaccharides and bioactive compounds that stimulate the main physiological processes of plants.

The aim of the work is to investigate the effect of the Algevit biostimulant on the content of vitamins A and C in *Momordica charantia* genotypes.

Following the determinations performed, a general trend of increasing the content of vitamins A and C was observed in all bitter cucumber genotypes after the application of the Algevit biostimulant, compared to the untreated controls. In the case of vitamin A, the values increased significantly, the highest concentration being recorded in the treated Linia 1 genotype (8.19 mg/100 g), with an increase of approximately 107% compared to the untreated control (3.95 mg/100 g). For vitamin C, the trend was similar, with the highest values also being obtained in treated Line 1 (23.69 mg/100 g), where an increase of about 57% was observed compared to the control (15.05 mg/100 g). The most pronounced percentage differences between the control and the treatment were therefore recorded in the same genotype, suggesting a high response capacity to the application of the biostimulator. These results were confirmed by the strong positive correlations within the Pearson correlation matrix.

References

1. Czompa A; Gyongyosi A; Szoke K; Bak I; Csepanyi E; Haines DD; et al. Effects of momordica charantia (Bitter Melon) on Ischemic Diabetic Myocardium. Molecules 2017 , 22(3). DOI: 10.3390/molecules22030488
2. Joseph B; Jini D. Antidiabetic effects of Momordica charantia (bitter melon) and its medicinal potency. Asian Pacific J Trop Dis 2013 , 3(2):93–102,. DOI: 10.1016/S2222-1808(13)60052-3
3. Abascal K; Yarnell E. Using bitter melon to treat diabetes. Altern Compl Ther 2005.
4. Barker T. Vitamins and Human Health: Systematic Reviews and Original Research. Nutrients 2023 , 15(13):15–18,.
5. Sung Goo K; Ashari S; Basuki N; Sugiharto AN. The Bitter Gourd Momordica charantia L.: Morphological Aspects, Charantin and Vitamin C Contents. IOSR J Agric Vet Sci 2016 , 09(10):76–81,. DOI: 10.9790/2380-0910017681

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PP5.25

Biotechnological production of ethanol from vegetable waste

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In recent years, the increasing demand for bioethanol has driven the search for alternative raw materials to traditional crops such as wheat, sugarcane, corn, and sugar beet, whose use often competes with the food industry. Vegetable waste has emerged as a promising substitute, offering a low-cost feedstock rich in fermentable sugars with high potential for bioconversion. Moreover, its utilization contributes to reducing environmental impacts, addressing one of today's pressing global challenges.

In this study, the valorization potential of potato, carrot, onion and cabbage wastes and their mixtures was studied by analyzing the composition of the substrates and determining the conversion yields to bioethanol as well as the efficiency of applying the sorting operation of this waste.

After studying the composition of these wastes, the presence of significant amounts of fermentable sugars was confirmed, such as: potato waste - 68%; carrot waste - 85%; onion waste – 88%; cabbage waste – 82%, and the compositions obtained were comparable to those identified in the literature, confirming the viability of these substrates as alternative sources for bioethanol production [1,2].

During the fermentation process, the residual glucose concentration in the bio-mixture was measured daily in order to track substrate utilization. This systematic monitoring served as a reliable indicator for identifying the end point of fermentation, which was reached after 4 days.

Bioethanol yields showed notable variations depending on the type of waste substrate employed. The highest conversion was achieved with carrot waste - 40.87%, followed by cabbage waste - 15.55%, onion waste - 13.2%, mixed waste - 10.2%, and potato waste - 6.7%. These results highlight carrot waste as a particularly efficient feedstock for ethanol production. Furthermore, implementing a waste sorting step improved overall yields, underscoring its technological and economic relevance.

A material balance was prepared for each process of ethanol production from waste. The highest mass loss was recorded for the process using cabbage waste – 36,96 g, while the lowest was observed for carrot waste – 11,86 g. Since glucose consumption was monitored throughout the process, it can be concluded that these losses were caused by its utilization in other metabolic pathways.

This research confirms the feasibility of producing ethanol from vegetable waste, demonstrating its potential as an alternative feedstock to conventional raw materials. To further increase ethanol yields, optimization of process parameters is required in order to maximize carbohydrate conversion into ethanol. Equally important is maintaining strict sterility throughout fermentation to avoid microbial contamination and ensuring the use of pure biocatalyst cultures to guarantee process stability.

References

1. ARAPOGLOU, D., VARZAKAS, T., VLYSSIDES, A., ISRAILIDES, C. Ethanol production from potato peel waste (PPW). In: Waste Management, 2010, vol. 30, nr. 10, pp. 1898–1902.
2. IFESAN, B. Chemical Composition of Onion Peel (Allium cepa) and its Ability to Serve as a Preservative in Cooked Beef. In: Human Journals, 2017, vol. 7, pp. 25-34.

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PP5.26

Exploring consumer preferences of plant-based alternatives: Insights from a Moldavian study

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Changing dietary habits towards a reduction of animal origin proteins in favor of plant-based food (PBF) alternatives can positively contribute to sustainability, health and animal suffering related issues [1, 2]. The present study of 187 Moldavian consumers examined plant-based food as substitute for animal-based food. Most of the respondents (58.1%) claimed that they have intermediate knowledge about PBF. Almost all respondents revealed a desire to improve their knowledge and to include PBF in their diet. Important factor in purchase decision was positive effect on health and environment ($p<0.05$). Therefore, reducing price, improving taste and availability taste are ways to reduce barriers to PBF consumption. Figure 1 shows the respondent's preferred PBF products.

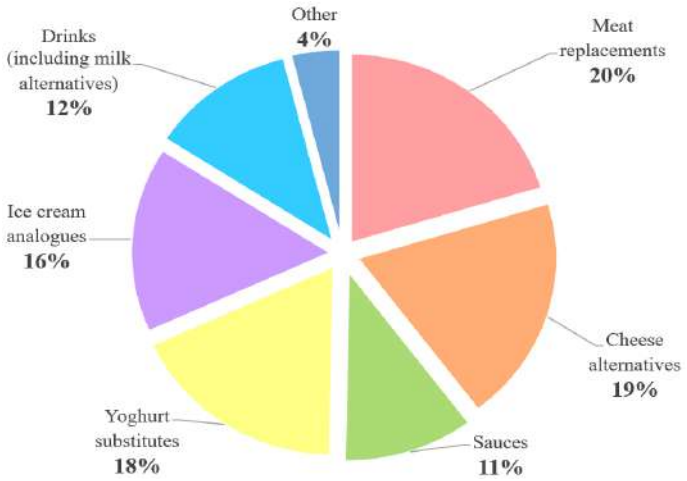

Figure 1. Distribution consumers concern on the preferred plant-based alternatives

Analysis showed that interest towards PBF did not differ between genders, but between participant's age, education and diet ($p<0.05$). Initiatives to improve public understanding of ways in which plant-based and animal-based products differ are also important, as many respondents were unclear about characteristics they associate with the two products.

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References

1. Granato, G., Wassmann, B. To imitate or not to imitate? How consumers perceive animal origin products and plant-based alternatives imitating minimally processed vs ultra-processed food. In: Journal of Cleaner Production, 2024, Vol. 472, 143447.
2. Popovici, C., Teng, X.M., Jadeja, R. Walnut cheese-like alternatives as an innovation among dairy analogues. In: Journal of EcoAgriTourism, 2024, Vol. 20, no. 2(49), 5-12 p.

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PP5.27

Walnut agricultural waste to value added bioactive compounds

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Walnuts by-products produced in large quantities after processing operations such as harvesting, hulling, drying and shelling are often underestimated and underutilized, wasting in their potential value [1]. Valorization of walnut by-products can increase the profitability of walnut processers and lead to several environmental and socioeconomic benefits [2]. This study was aimed to apply Soxhlet extraction (SE) method to recover bioactive compounds from walnut leaves, green husks, and wooden membrane septum, to identify their chemical nature and to evaluate antioxidant potential.

Walnut by-products have been dried, packed and grounded before extraction. The dried powder has been extracted with water, ethanol and their mixtures at different concentrations from 0% to 100% EtOH for 2 h at 60 ºC and solid to liquid ratio 1 g per 10 ml of solvent. The produced extracts have been analyzed using UV/Vis spectra and evaluated in terms of extraction yields, $DPPH^{\bullet}$ and ABTS antioxidant activity, total polyphenol and flavonoid compounds.

The integrated image of bioactive compounds composition and the differences between their concentrations in walnut by-products have been identified. The studied extracts displayed strong peaks, typical for phenolic acids (237 and 290 nm), flavonoids (333 nm) and carotenoids (417, 457, 484 and 538 nm). The $DPPH^{\cdot}$ and ABTS values of the tested extracts have been in the range of 54.25 – 83.31% for walnut leaves extracts, 44.21 – 65.73% for walnut green husks extracts and 85.72 – 95.34% for wooden membrane septum extracts. The optimal solvent for bioactive compounds extraction from walnut leaves was identified as 70%, from walnut green husks as 50% and from walnut membrane septum as 30% mixture of water and ethanol.

The results of the present study suggest that walnut leaves, green husk and membrane septum extracts, by-products of walnut processing industry, can be utilized as an economical source of natural antioxidants for food, cosmetic and pharmaceutical industries.

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References

1. Paşayeva, L., Yetimoğlu, S., Fatullayev, H., İnce, U., Bozkurt, N.M., Karaboğa Arslan, A.K. Optimizing health benefits of walnut (*Juglans regia* L.) agricultural by-products: Impact of maceration and Soxhlet extraction methods on phytochemical composition, enzyme inhibition, antioxidant, antimicrobial, and cytotoxic activities. In: Food Bioscience, 2025, Vol. 64, 105923, ISSN 2212-4292.
2. opovici, C. Soxhlet extraction and characterisation of natural compounds from walnut (*Juglans regia* L.) by-products. In: Ukrainian Food Journal, Vol. 2, Is. 3, ISSN 2304-974X, p. 328 – 336.

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PP5.28

Biological protection of plants in strengthening the "One Health" concept

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Globally, the worsening of the phytosanitary condition, the environment and the health status of biological entities is increasingly being recorded. The increase in losses caused by pests against the background of climate change, which lies in the modification of the invasive and epidemiological particularities of phytosanitary agents and the increase in the prevalence of pests through the presence of various difficulties in carrying out the technological processes for the production of agricultural crops. The need to ensure:

- the broad implementation of biological plant protection as an approach to plant health that respects the environment and creates conditions for the promotion of ecological agriculture;
- the harmonious combination of the results recorded with the practice of integrated plant protection, especially with the aim of obtaining ecologic products;
- promoting complex prophylactic measures and implementing scientific results in the unitary legislative system in order to protect the health of the human population;
- determination of the mechanisms and links between soil, plant, animal and human health.

The following achievements have been recognized: the development of technological processes for the production of 15 entomophages, especially those applied in the protection of crops in protected areas; selection of prospect microorganisms and development of technologies for the production and application of microbiological agents to control harmful organisms and approval based on them of 16 biological preparations; identification and synthesis of sexual pheromones of 18 species of harmful insects and elaboration of original pheromone synthesis schemes in 72 species and of the technological processes for their production and use for monitoring, mass capture, sterilization and disorientation of pests. Biological plant protection products are effective means of preserving the health of plants, animals, humans and soil biota with positive effects on biodiversity and ecosystems, helping to ensure the resilience of agriculture. The results recorded and the implementation of biological plant protection strengthen the health of biological entities and reveal the driving forces behind a faulty protection system, proposing a path oriented towards building true resilience of plants, animals, biological diversity and human health.

In solving technological problems for the protection of plant health, there is a strengthening of the "One Health" concept at global level by implementing the global strategy of expanding interdisciplinary collaborations and communications in all aspects related to the preservation of human, plant, domestic animal or wildlife health, which can no longer be tackled separately, but only jointly, inherent. This relates not only to concerns about regulating the density of pest populations, but also to lifestyle issues, diet, the impact of different types of human-animal-plant-soil relationships, and exposures, which can affect all population categories.

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PP5.29

Productive potential of *Saccharomyces* yeasts and antifungal properties of their exopolysaccharides

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Yeasts, especially those of the genus *Saccharomyces*, represent a natural source of various biologically active substances [1], recognized as safe (GRAS) for human consumption [2]. The biomass of *Saccharomyces* yeasts and their derived products are rich in proteins, essential and immunoactive amino acids, carbohydrates and polysaccharides. They possess nutritional value, antioxidant, antimicrobial, immunostimulatory, and anti-inflammatory properties, and are widely used in the food industry, cosmetology, veterinary science and medicine.

The aim of this research was to evaluate the possibility of using natural nutrient media, obtained from agro-industrial wastes of barley (BaE), carrot (CE) and red beet (BE), as the single source of nutrition for cultivating *Saccharomyces* yeasts, obtaining biomass and producing biologically active products. Four *Saccharomyces* strains, such as *Saccharomyces sp*. 7, *Saccharomyces sp*. 9, *Saccharomyces sp.* 10 and *Saccharomyces sp*. 11 isolated in pure culture from different artisanal bakery sourdough were used in the study. At the end of the submerged cultivation cycle of 120 hours, at the temperature of +27-28°C with continuous agitation at 200 rpm, the biomass productivity of the strains, their biochemical composition, the exopolysaccharide content in the culture liquid and their antimicrobial activity were determined.

It was established that the strains produced from 8.02±0.46 to 9.24±0.21 g/L dry biomass on the BaE medium, from 6.46±0.31 to 7.86±0.11 g/L on the CE medium, and from 7.11±0.22 to 11.07±0.02 g/L on the BE medium, which is significantly more compared to the productivity of these strains on the classic YPD medium, used as a control. The yeast biomass cultivated on these natural nutrient media possess antioxidant activity, activity of CAT and SOD enzymes, and contain significant amounts of proteins and carbohydrates.

The strains also synthesized and secreted considerable amounts of exopolysaccharides into the culture liquid. Thus, the studied strains produced of 2.04±0.02-4.19±0.32 g/L exopolysaccharides on the BaE medium, of 4.33±0.27-5.72±0.22 g/L on the CE medium, and of 5.55±0.46-7.37±0.91 g/L on the BE medium. Exopolysaccharide solutions of varying concentrations, obtained from CE and BE nutrient media, exhibited significant antifungal activity against different strains of fungi (*Aspergillus flavus, Aspergillus fumigatus, Fusarium oxysporum*), with inhibition zones of the tested strains ranging from 27.0±2.64 to 43.66±1.52 mm.

In conclusion, it can be mentioned that exopolysaccharides of the *Saccharomyces* yeasts, isolated from various artisanal bakery sourdough and cultivated on natural media derived from barley, carrot and red beet residues, possess significant antifungal activity and potential for application in various fields, including veterinary science and medicine.

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References

1. Doolam, B., Mishra, B., Surabhi, D., et al. (2024). A systematic review of potential bioactive compounds from Saccharomyces cerevisiae: exploring their applications in health promotion and food development. Environment, Development and Sustainability. 1-38.

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PP5.30

Technological and functional potential of cereal and legume flours for the formulation of fermented food prototypes

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The increasing consumer demand for functional foods has driven research towards the valorization of alternative plant raw materials as substrates for fermentation. Cereal and legume flours represent promising candidates due to their nutritional density, high protein content, dietary fiber, and bioactive compounds that can be enhanced through microbial biotransformation. The present study aimed to characterize the technological and functional potential of selected cereal (oats, rye) and legume (chickpea, lentila) flours as substrates for the formulation of fermented food prototypes.

A comprehensive set of analyses was carried out to evaluate both the nutritional composition and functional attributes of the raw materials. Proximate composition was determined by standard methods: moisture (gravimetric), protein (Kjeldahl), fat (Soxhlet), ash (muffle furnace), carbohydrate content (by difference), and dietary fiber (enzymatic-gravimetric). The bioactive profile was assessed through quantification of total polyphenols (Folin–Ciocalteu assay), flavonoids ($AlCl_3$ colorimetric method), and antioxidant capacity (DPPH and ABTS radical scavenging assays). In parallel, technological properties relevant for fermentation were investigated, including water absorption capacity, water retention capacity, swelling index, and hydration properties. The results demonstrated substantial variability between cereal and legume flours. Legume-based flours exhibited higher protein levels (18–24%) compared to cereal flours (10–14%), confirming their potential to improve the amino acid balance of fermented formulations. Conversely, cereal flours presented higher carbohydrate and starch fractions (55–65%)**,** favoring microbial growth and lactic acid production. Total polyphenol content ranged between 120–240 mg GAE/100 g d.m.**,** with legumes generally exhibiting higher levels than cereals. Antioxidant activity followed a similar trend, suggesting that legume substrates could deliver an additional functional benefit through enhanced radical scavenging capacity. Hydration properties varied significantly: chickpea and lentil flours showed water absorption values exceeding 200%**,** whereas rye and barley flours exhibited lower but more stable swelling indices. These functional differences are crucial in tailoring fermentation protocols, since water availability and substrate consistency directly influence microbial viability and metabolite production.

From a technological perspective, the combined analysis indicated that mixed formulations of cereal and legume flours could provide balanced nutritional and functional properties**,** while mitigating the individual limitations of each group (e.g., low protein in cereals vs. reduced starch availability in legumes). These findings underline the suitability of both cereals and legumes as fermentation substrates and establish a rational basis for selecting raw materials in the development of functional fermented food prototypes.

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PP5.31

Stability and functionality of liposomes as carriers of polyphenols in foods

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The fortification of foods with bioactive compounds is a major trend in functional food development, aiming to provide health benefits beyond basic nutrition. Polyphenols, abundant in plant sources, are recognized for their strong antioxidant, anti-inflammatory, and cardioprotective properties. Despite their remarkable bioactivity, their direct incorporation into foods is limited by poor solubility, low stability under processing and storage conditions, and reduced bioavailability in the gastrointestinal tract. Liposomal encapsulation represents a promising delivery strategy to overcome these limitations, offering enhanced stability, protection against oxidative degradation, and improved release profiles of polyphenols.

In this study, polyphenol-rich extracts were successfully encapsulated into liposomes using an adapted method after Mozafari [1]. The resulting liposomal formulations showed desirable physicochemical properties, with particle sizes up to 200 nm, ensuring nanoscale dispersion and compatibility with diverse food matrices. Encapsulation efficiency exceeded 90%, confirming the ability of liposomes to entrap and retain high amounts of polyphenolic compounds. Stability tests further demonstrated that liposomes preserved the antioxidant potential of polyphenols over time, while maintaining structural integrity during simulated processing and storage.

The results highlight liposomes as multifunctional carriers that not only stabilize polyphenols but also enhance their nutritional and functional impact when incorporated into foods. Their applicability extends across bakery, dairy, meat, plant-based, and beverage products, where they can improve oxidative stability, prolong shelf life, and deliver health-promoting compounds more efficiently. These findings provide valuable insights into the use of liposomal systems as sustainable fortification strategies, aligning with consumer demand for innovative and health-oriented food products.

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References

1. Rasti, B.; Jinap, S.; Mozafari, M.R.; Yazid, A.M. Comparative Study of the Oxidative and Physical Stability of Liposomal and Nanoliposomal Polyunsaturated Fatty Acids Prepared with Conventional and Mozafari Methods. Food Chem. 2012, 135, 2761–2770.

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PP5.32

Fortification strategies of food products using carotenoid-loaded liposomes

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Food safety is a key concern for consumers and the food industry, as oxidative degradation of biomolecules contributes to the onset of chronic diseases such as cancer, cardiovascular disorders, cataracts, and diabetes. Natural antioxidants, particularly carotenoids, play an important role in preventing oxidation and extending the shelf life of food products. However, their application is limited due to poor stability and low bioavailability. Liposomal encapsulation emerges as an effective strategy to overcome these challenges by protecting carotenoids from oxidative degradation, enhancing their stability, and improving their delivery in food matrices.

In this study, carotenoid-rich lipophilic extracts from sea buckthorn were successfully encapsulated into liposomes using an adapted heating method. The liposomal formulations demonstrated high encapsulation efficiency, strong retention of bioactive compounds, and improved antioxidant potential. Incorporation of carotenoid-loaded liposomes into food products such as biscuits revealed promising results in terms of maintaining nutritional and functional properties during processing and storage. Results showed that water-based liposomes exhibited the highest encapsulation efficiency (92.12±1.32%), retention rate (88.92±2.52%), and encapsulated bioactive compound content (89.14±6.52μg), confirming their superior performance compared to other formulations.

These findings highlight the potential of carotenoid-loaded liposomes as a fortification strategy for a wide range of food products, including bakery, dairy, meat, plant-based alternatives, and beverages. Their application not only improves the oxidative stability and bioavailability of carotenoids but also contributes to the development of functional foods with added health value. Overall, liposomal encapsulation represents a sustainable and innovative approach that aligns with consumer demand for healthier, more stable, and nutritionally enhanced food products.

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PP5.33

Residual yeasts from winemaking: A valuable source of biologically active substances with multifunctional properties

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In the wine industry of the Republic of Moldova, residual yeast represents a substantial but underexploited resource. Currently, this by-product is frequently discarded or employed in limited ways, such as ethanol production or soil fertilization. Nevertheless, residual yeast is a rich source of bioactive compounds, including proteins, polysaccharides, polyphenols, and minerals. Among these, β-glucans occupy a prominent position due to their complex structure and well-documented multifunctional properties, such as immunomodulatory, antioxidant, and texturizing effects. These attributes make them particularly attractive for applications in the food, pharmaceutical, and cosmetic industries.

The purpose of this study was to investigate the most effective extraction method for β-glucans derived from the biomass of residual wine yeasts originating from local grape varieties. Several extraction techniques—mechanical, enzymatic, chemical, and combined approaches—were comparatively analyzed to evaluate their impact on the purity, yield, and physicochemical properties of the isolated β-glucans. The results revealed that the applied extraction method significantly influences not only the efficiency of recovery but also the structural integrity and functional characteristics of the obtained compounds.

The findings confirm that residual wine yeast is not merely a waste product but a valuable raw material for obtaining high-quality β-glucans with multifunctional applications. Their integration into innovative food formulations could enhance nutritional and technological value, while potential uses in biomedical and cosmetic fields further expand their importance. Moreover, the sustainable valorization of this secondary stream aligns with the principles of the circular economy by reducing winery waste and generating high-value products.

This study provides new insights into optimizing the biotechnological potential of residual yeast in the Moldovan wine sector, demonstrating how an underutilized resource can be transformed into a source of bioactive compounds with significant industrial and societal relevance.

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References

1. Chioru, A., Chirsanova, A., Dabija, A., Avrămia, I., Boiștean, A., & Chetrariu, A. (2024). Extraction Methods and Characterization of β-Glucans from Yeast Lees of Wines Produced Using Different Technologies. Foods, 13(24), 3982. https://doi.org/10.3390/foods13243982
2. Trohina, A., Chirsanova, A., Boiștean, A. Rheological characteristics of beta-glucans obtained from wine lees of wines from local grapes varieties. In: The Biotechnologies, Present and Perspectives: intern. conf., 15 Dec. 2023, Suceava, Romania, 9 ed.: abstracts, Suceava, 2023, p. 21. ISSN 2068–0819. http://repository.utm.md/handle/5014/27183
3. Boiștean, A., Chirsanova, C. A., & Chioru, A. (2024). Producerea de β-glucan din drojdiile vinurilor locale produse cu utilizarea diferitor tehnologii. In: Conferința Științifică Națională "Inovația: Factor Al Dezvoltării Social-Economice", Cahul, Republica Moldova, Ediția a IX- a, 12 Decembrie, 2024. Universitatea de Stat "Bogdan Petriceicu Hasdeu" din Cahul. Cahul: Print-Caro, 2024, pp. 45-46. ISBN 978-9975-88-128-9. https://repository.utm.md/handle/5014/31857

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PP5.34

Microbial strains with antifungal properties

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Microorganisms are widespread everywhere in nature (water, soil, air, on the surface and inside plants and all living things). They actively participate in the cycle of matter in nature, the decomposition of various organic and inorganic materials, in the formation and fertilization of soil, the carbon cycle in nature, etc. Microorganisms are widely used in biotechnology to obtain various bioactive products (vaccines, antibiotics, vitamins, enzymes, food additives, biofertilizers, phytostimulants, insecticides, antimicrobial products, organic acids, etc.). Microorganisms can also cause various diseases in all living beings (plants, animals, humans). To treat these diseases, antimicrobials are most often used, but their excessive and abusive use leads to the emergence of resistance to antimicrobials, the majority of which are obtained on the basis of microorganisms. The study focused on the selection of microbial strains with high antimicrobial capacities is necessary and current. Thus, the purpose of the research was to select microbial strains with high potential for the synthesis of antifungal substances useful for medicine.

To achieve this goal, a screening of 31 microbial strains (24 strains of micromycetes and 7 strains of actinobacteria) was carried out for their antifungal capacity against opportunistic pathogens: *A. fumigatus*, *F. solani*, *F. oxysporum* and the pathogen *Candida albicans*.

The tests were carried out according to the disk diffusion method by Egorov, 2004.

Malt-agar medium served as the cultivation medium for micromycetes strains, and Gause medium for actinobacteria.

The study results showed that 2 strains of fungi (*Penicillium* sp. 12 and *Penicillium* sp. 14) and 2 strains of actinobacteria (*Streptomyces gougerotii* CNMN-Ac-14 *and Streptomyces fradiae* CNMN-Ac-11) show antagonism towards opportunistic pathogens: *A. fumigatus*, *F. oxysporum*, *F. solani* with inhibition zones of 20-30 mm, and the strain *Penicillium* sp. 12 and *Streptomyces fradiae* CNMN-Ac-11, also showed antagonism towards *Candida albicans* (inhibition zones of 14-15 mm).

Testing of Fe_2O_3; Fe_2ZnO_4 nanoparticles (NP) in concentrations of 1, 5, 10 mg/l and barley extract as stimulators of the biosynthesis of bioactive components in the selected strains: *Penicillium* sp. 12 and *Streptomyces fradiae* CNMN-Ac-11 did not give positive results. The most significant results, compared to the tested pathogens, were obtained in the control variant.

Thus, the results obtained demonstrated that the *Penicillium* sp. 12 and *Streptomyces fradiae* CNMN-Ac-11 strains possess antifungal properties against opportunistic pathogens: *A. fumigatus*, *F. solani*, *F. oxysporum* and the pathogen *Candida albicans*.

Research to stimulate the biosynthesis of bioactive components in the selected strains continues.

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Oleogels in the food industry: innovative solutions for healthy nutrition and sustainable development

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The modern food industry is at a crossroads, facing a dual challenge: meeting growing consumer demand for healthy products and reducing its environmental impact. In this context, the development of innovative ingredients that can improve the nutritional value of products without compromising their organoleptic and technological properties is of particular importance. One of the most promising areas is the use of oleogels – structured systems based on liquid vegetable oils that offer a revolutionary approach to replacing traditional solid fats rich in saturated and trans fatty acids [1,2].

Oleogelation is the process of converting liquid oils into semi-solid or solid structures by forming a three-dimensional network of oleogelating agents. These agents, including various waxes (beeswax, carnauba wax, rice bran), proteins (pea, soy) and polysaccharides (ethyl cellulose, xanthan gum), encapsulate the liquid oil, giving it the desired viscoelastic properties. The key advantages of oleogels that make them so attractive to the food industry include: improved nutritional value by replacing saturated and trans fats with unsaturated fatty acids contained in liquid vegetable oils, which helps reduce the risk of cardiovascular disease and improve the overall health of consumers [1,3]; functional equivalence, successfully mimicking the textural, rheological and stabilising properties of traditional solid fats [3]; increased oxidative stability, contributing to reduced oil oxidation and increased product shelf life; expansion of the range of specialised products to create products that meet specific dietary needs, such as gluten-free, lactose-free, vegan products, as well as products with reduced fat or sugar content, in line with current healthy eating trends; and effective delivery of biologically active compounds, serving as an ideal matrix for the encapsulation and controlled delivery of fat-soluble vitamins, antioxidants, probiotics and other valuable biologically active compounds. The potential applications of oleogels cover virtually all segments of the food industry. Future research in the field of oleogels is focused on the development of new, more effective and environmentally friendly oleogelling agents, including those derived from food industry by-products.

Keywords: oleogelling agents, structured systems, encapsulation, functional food.

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References

1. PUȘCAȘ, A., MUREȘAN, V., SOCACIU, C., & MUSTE, S. OLEOGELS IN FOOD: A REVIEW OF CURRENT AND POTENTIAL APPLICATIONS. IN: *FOODS*, 2020, *9*(1), 70. HTTPS://WWW.MDPI.COM/2304-8158/9/1/70
2. MANZOOR, S., MASOODI, F., NAQASH, F., RASHID, R. OLEOGELS: PROMISING ALTERNATIVES TO SOLID FATS FOR FOOD APPLICATIONS. IN: *FOOD HYDROCOLLOIDS FOR HEALTH*, 2022, *2*, 100058. HTTPS://DOI.ORG/10.1016/J.FHFH.2022.100058
3. LIU, L., GAO, Z., CHEN, G., YAO, J., ZHANG, X., QIU, X., LIU, L. A comprehensive review: Impact of oleogel application on food texture and sensory properties. In: *Food Sci Nutr.*, 2024 Apr 13;12(6):3849-3862. https://doi.org/10.1002/fsn3.4110

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PP5.36

Horseradish leaves – a new promising source for obtaining kaempferol

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Kaempferol (3,4′,5,7-tetrahydroxyflavone), along with quercetin, is the main representative of flavonol aglycones and is found, mainly in the form of glycosides, in many food and medicinal plants, with variable content (0.1-832 mg/kg) [1, 2]. It has a wide range of pharmacological effects: antibacterial, antifungal, anti-inflammatory, antioxidant, cardioprotective, antidiabetic, and others [1, 2]. Kaempferol glycosides, mainly rustoside, are contained in the leaves of such a widespread and industrially cultivated plant as horseradish [3], but we did not find any mention of using horseradish to obtain kaempferol.

This study evaluated horseradish leaves as a potential source of kaempferol. Horseradish leaf samples were collected from the spontaneous flora of the central part of the Republic of Moldova, air-dried and crushed to a particle size of no more than 0.4 mm. The analysis was performed by HPLC with diode-array detection after extracting the samples with 60% ethanol for an hour at 60°C. Since there was no commercially available rustoside standard, we performed hydrolysis of the glycosides by heating the extracts, acidified with hydrochloric acid to a concentration of 0.2 M, for 2 h at 80°C, followed by determination of kaempferol. The maximum recovery of kaempferol was obtained at HCl concentrations of 0.15 - 0.25 M. Concentrations above 0.3 - 0.5 M lead to noticeable destruction of kaempferol, and concentrations below 0.1 M require too long a heating time. The kaempferol content, found in horseradish leaves, reached its maximum in early June and varied from 29 to 52 mg/g depending on the growing location, averaging 37 ± 6 mg/g. This is significantly higher than in most plant species used so far for the isolation of kaempferol. Higher kaempferol content was observed in young leaves. We also found a more than 2.5-fold range of variation in this indicator when analyzing individual plants taken from one population. Thus, given the above values and the availability of plant material, horseradish leaves should be considered a very promising natural source for the industrial production of kaempferol with a yield of up to 35-40 grams per kilogram of raw material (theoretical values), and the low hydrolytic stability of rustoside helps to reduce the material and energy intensity of production.

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References

1. Jan, R.; Khan, M.; Asaf, S. Et al. Bioactivity and Therapeutic Potential of Kaempferol and Quercetin: New Insights for Plant and Human Health. Plants 2022, 11, 2623. https://doi.org/10.3390/plants11192623
2. Li Yang, Y. Gao, V. K. Bajpai et al. (2021): Advance toward isolation, extraction, metabolism and health benefits of kaempferol, a major dietary flavonoid with future perspectives, Critical Reviews in Food Science and Nutrition 63(16): 2773-2789. DOI: 10.1080/10408398.2021.1980762
3. N. Fursa, V. Litvinenko. Rustoside from Armoracia rusticana. Chem Nat Compd 6, 657 (1970). https://doi.org/10.1007/BF00563477

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PP5.37

HPLC-MS analysis of phenolic compounds in *Solidago* species from the flora of the Republic of Moldova

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Introduction. Species of the genus *Solidago* (goldenrods) are particularly rich in phenolic constituents, including flavonoids and phenolic acids. These metabolites have been associated with antioxidant, anti-inflammatory, and cytoprotective effects, supporting the traditional use of *Solidago* extracts in folk medicine for urinary tract disorders and inflammatory conditions.
Purpose of the work. The identification and quantification of key phenolic compounds in dry extracts of Solidago species from Moldovan flora by high-performance liquid chromatography (HPLC) coupled with mass spectrometry (MS).
Material and methods. The aerial parts of *S. virgaurea* and *S. canadensis* plant species were collected from the flora of the Republic of Moldova. Polyphenols were extracted with 60% ethyl alcohol, by the fractional maceration method, while the dried extracts were concentrated using a Laborota 4011 rotary evaporator. For the HPLC analysis, an Agilent 1200 HPLC system was used, equipped with a quaternary pump, solvent degasser, autosampler, UV-Vis photodiode array detector (DAD) coupled with a single quadrupole mass detector (MS), Agilent model 6110. For the MS, the positive ESI full-scan ionization mode was used under the following operating conditions: capillary voltage 3000 V, temperature 350°C, nitrogen flow rate 7 L/min, and m/z range 120–1200.
Results. Phytochemical investigations of goldenrods dry extracts using HPLC–MS have revealed that the extract of *S. canadensis* exhibited a higher content (µg/mg DW) of phenolic compounds (390.712) compared to *S. virgaurea* (259.778). A complex phenolic profile is dominated by flavonols from flavonoids and some phenolic acids. Thus, the extract of *S. canadensis* showed a higher content (µg/mg DW) and a broader range of flavonoid compounds, including rutin (73.210), kaempferol-acetyl-glucoside (52.142), isorhamnetin-rutinoside (21.586), quercetin (14.367), and isoquercitrin (12.933). On the other hand, the extract of *S. virgaurea* was distinguished by the representative flavonoids, as follows: rutin (38.483), kaempferol-rutinoside (28.299), hyperoside (14.767), and isoquercitrin (13.408), while notable phenolic acids comprise chlorogenic acid (53.020), syringic acid (49.943), and 3,5-dicaffeoylquinic acid (30.023). It is important to note that hyperoside was identified exclusively in the extract of *S. virgaurea*, whereas isorhamnetin-rutinoside and quercetin-acetyl-glucoside were detected only in the extract of *S. canadensis*, which indicates that these compounds may be considered specific markers for the respective *Solidago* species.
Conclusions. The HPLC-MS analysis of phenolic compounds in *Solidago* species demonstrated that they are rich sources of phenolic metabolites. Among them, *S. canadensis* was distinguished by a higher content, which underscores the need for further phytochemical and pharmacological investigations, highlighting their potential as valuable sources of bioactive compounds.
Keywords: *Solidago* species, Republic of Moldova flora, phenolics, HPLC-MS analysis
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PP5.38

Comprehensive monitoring of pesticide residues in Romanian fresh products

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The intensification of global agriculture has led to widespread pesticide use, raising concerns about impacts on human health and the environment. This study investigates the occurrence and levels of pesticide residues in fruits and vegetables from Romanian markets. A total of 620 randomly selected horticultural samples were analysed for 74 authorized pesticides using the QuEChERS extraction method and LC–MS/MS. Boscalid and azoxystrobin were the most frequently detected compounds, present in 42% of apple and 37% of strawberry samples, with mean concentrations of 0.12 mg/kg and 0.09 mg/kg, respectively. In cucumbers and tomatoes, difenoconazole and acetamiprid predominated (35% and 40% of samples; 0.08 and 0.07 mg/kg on average). The results showed significant variations in residue levels by product type and origin. While most residues complied with EU maximum residue limits (MRLs), 6% of samples—mainly imported—approached or exceeded critical thresholds, particularly for chlorpyrifos and lambda-cyhalothrin (up to 0.25 mg/kg). These findings provide a data-driven overview of pesticide contamination in Romania's fresh produce supply, supporting consumer awareness and emphasizing the need for continuous monitoring and reinforced food safety regulations.

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PP5.39

Chemistry in service of nutrition: Multi-marker profiling of raspberries for safe and functional food development

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Stable isotope and phenolic analysis are powerful tools at the interface of chemistry, agriculture and medicine, enabling food traceability, authenticity verification and insights into nutritional quality. Within the European Green Deal and Farm-to-Fork strategy, raspberries represent a valuable case study for demonstrating how chemical markers can be translated into healthier diets and sustainable agri-food systems. In this study, two cultivars (*Opal* and *Delniwa*) were investigated under contrasting cultivation systems: agroforestry and organic plantation. Both were compared with commercial raspberries produced conventionally. Field plots were further divided into control and biofertilizer lots, receiving either a digestate derived from corn–soy–sorghum (SOBIOSUS) or a composite amendment of dolomite, slag, CKD, grape pomace and yeast (InnES).

A comprehensive compositional fingerprint was established by combining elemental analysis, extended phenolic profiling and stable isotope ratios ($\delta^{13}C$, $\delta^{15}N$, $\delta^{2}H$, $\delta^{18}O$). Results demonstrated clear discrimination between cultivars and production systems, with biofertilization strategies enhancing functional compounds such as rutin, quercetin, chlorogenic and ellagic acids while maintaining food safety. Isotopic markers provided robust signatures of cultivation environment and fertilization input, complementing nutritional descriptors. Together, these markers revealed how eco-friendly practices can improve fruit resilience, nutritional functionality and authenticity.

The results revealed consistent differences between cultivars and production systems. *Opal* and *Delniwa* separated along mineral–phenolic axes, while agroforestry and organic plantations showed distinct isotopic windows. $\delta^{13}C$ values ranged between –27.5 ‰ and –22.9 ‰, $\delta^{15}N$ spanned from negative values to over +8 ‰, and $\delta^{2}H$ and $\delta^{18}O$ displayed broad variability reflecting environmental conditions. Biofertilization significantly modulated fruit quality: InnES amendments enhanced chlorogenic and ellagic acid content, whereas SOBIOSUS digestate promoted increases in flavonoids such as rutin and quercetin. In most cases, biofertilization was associated with elevated antioxidant capacity without compromising safety indicators. Market samples, in contrast, clustered in narrower isotopic and phenolic ranges, suggesting standardization of inputs and processing.

By translating analytical chemistry into nutritional insights, this work highlights the role of isotopic and phenolic profiling in bridging primary production with human health. These findings support the development of reliable traceability and authentication tools for berry-based value chains. More broadly, they illustrate how eco-friendly fertilization strategies can improve fruit quality and resilience without increasing environmental risks.

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PP5.40

Extended reproducibility assessment for metabolomics experiments

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Metabolomics has become an important topic in a wide range of scientific areas, including medicine, pharmacology, nutrition and metabolism, food sciences and environmental research. As metabolomics requires processing of large numbers of multiple parameters, the reproducibility of data for statistical purposes is a key issue. Recent studies shown impressive interlaboratory reproducibility of NMR spectra, but such studies involved trained personnel and standardised solutions. As metabolomics became an established topic in education, the NMR metabolomics penetrated in several research laboratories with a wide range of backgrounds and research interests. The purpose of the present study was to evaluate the NMR reproducibility for metabolomics in a "real-life" situation when combining both industry-standard NMR solutions and multipurpose NMR equipment, and to compare the reliability of NMR metabolomics data when involving both dedicated NMR operators (including researchers and technicians) and chemistry users from outside the NMR group (including researchers and students). An interlaboratory assessment of NMR quantitation reproducibility was performed using two NMR instruments and involving several operators with different backgrounds and metabolomics expertise. The variability induced by operator, automatic pipettes, NMR tubes and NMR instruments was evaluated in order to assess the limiting factors for quantitation reproducibility. The results estimate the expected reproducibility data in a real-life multipurpose NMR laboratory.

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PP5.41

Study of high protein biological matrices by NMR spectroscopy

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NMR spectroscopy has proven to be valuable tools in the study of human and animal metabolism. By identifying and quantifying metabolites, information into the biochemical pathways and mechanisms underlying diseases can be obtained. Widely recognized for the capacity to offer structural information through non-destructive, reproducible and quantifiable analysis, NMR continues to be the method of choice for metabolomic investigation.

Blood plasma/serum, urine, milk and tissue are among the most commonly used biological matrices in the metabolomics field. Both serum and plasma, easily obtained after blood centrifugation, contain metabolites and proteins. Many different factors, such as genetics, age, sex, diet and lifestyle, can affect the metabolic composition. Additionally, pre-analytical factors like the collection and storage conditions of serum or plasma specimens can significantly affect metabolite concentrations. Lipoprotein profiling of plasma samples without extraction, can be useful for the study of diseases. The deconvolution of the methyl signal is associated with each lipoprotein subtype: large, medium and small of the main types of lipoprotein—very low density lipoprotein (VLDL), low density lipoprotein (LDL) and high density lipoprotein (HDL).

^{1}H NMR of milk samples has been used to in monitoring animal health and metabolic status. Milk samples can be analyzed without pretreatment or after lipids removal by centrifugation and/or protein precipitation.

In this study, several samples of fresh cow milk and serum were analyzed through NMR spectroscopy. The characteristic NMR profiles for these biofluids are presented in **figure 1**.

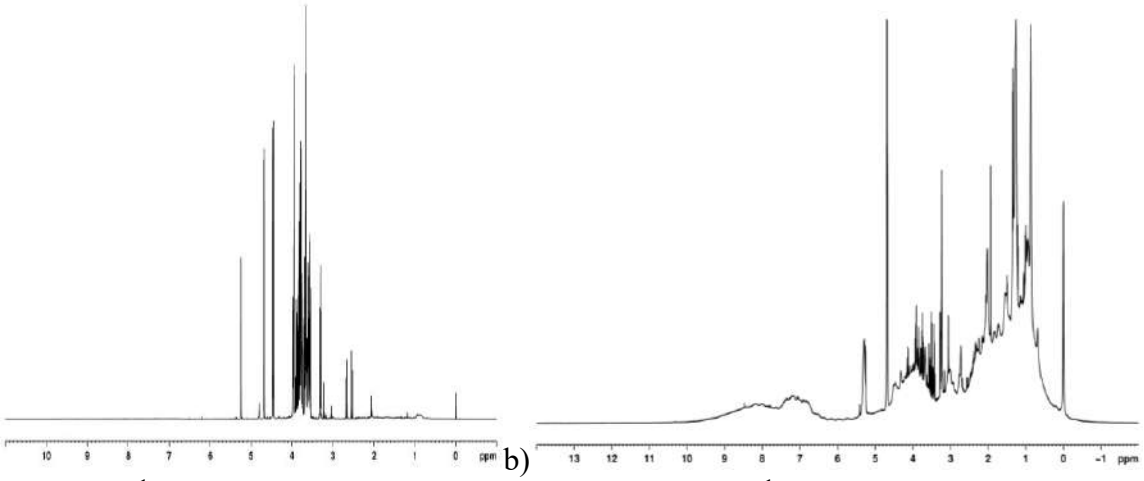

Figure 1. a) ^{1}H NMR spectrum of fresh cow milk sample; b) ^{1}H NMR of cow serum.

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Targeting Chronic Wound Pathogens with Sulfonamide-Enhanced Nitrogen Scaffolds

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Chronic wounds present a persistent clinical challenge, frequently complicated by polymicrobial infections and the emergence of antimicrobial resistance (AMR). As the effectiveness of conventional antibiotics declines, there is a critical need for novel therapeutic agents that not only inhibit microbial growth but also address the oxidative stress that impairs wound healing. In this study, we report the design, synthesis, and biological evaluation of two novel series of sulfonamide derivatives featuring a pyrrol-2-one nitrogen scaffold, a structure known for its pharmacological versatility.

A total of 28 compounds were synthesized, incorporating sulfonamide substituents at either the *meta* (3-SA series) or *para* (4-SA series) positions on the phenyl ring. These derivatives were assessed for antimicrobial activity against clinically relevant chronic wound pathogens and results indicates that 3-SA series posses superior antimicrobial efficacy, with several compounds showing significant activity even against strains with known multidrug resistance profiles.

In parallel, antioxidant potential was evaluated using multiple assays, revealing that selected 3-SA derivatives also possess enhanced radical-scavenging capabilities. These findings highlight the therapeutic promise of meta-substituted sulfonamide-pyrrol-2-one hybrids as multifunctional agents that can simultaneously target microbial infection and oxidative damage in chronic wound environments. This dual-action profile underscores their potential for further development in advanced wound care strategies.

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PP5.43

Ceria-doped materials synthesis and characterization

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Cerium oxide, CeO_2, or simply ceria, has been extensively studied over the last few decades due to its unique redox properties and remarkable oxygen storage capacities.[1] CeO_2 materials have been synthesized in many forms, shapes, and sizes. Several companies worldwide produce CeO_2, which is commonly used in various applications, including polishing, electronics, glass manufacturing, and catalysis.

Despite the much-focused efforts by the scientific community, the preparation of ceria-based materials with sufficiently high surface area, high defect concentration, and high thermal stability is still incompletely controlled. [2] Therefore, is our duty to continue this effort, and based on our expertise, to develop the ceria-based materials synthesis. The principal scope of this study is to validate the precipitation route for ceria-doped materials and scale up the synthesis at laboratory scale, and to extend their applicability as catalysts for CO_2 reduction to added value products.

The materials were prepared by a modified co-precipitation route described elsewhere [2], and the Cu loadings were between 0.5 and 2%. The synthesized materials were characterized by N_2 adsorption-desorption volumetry, X-ray diffraction (XRD) to determine the crystalline phases of the powder catalysts, and temperature programmed reduction experiments (TPR-H_2) to determine the reduction degree. The Brunauer-Emmett-Teller (BET) method was used to calculate the specific surface area from the data obtained at P/P0 between 0.01 and 0.995.

The characterization data indicated that all samples show the typical diffraction pattern of the CeO_2 pure cubic fluorite structure, and by doping with Cu, the surface area of the ceria increased from 66 $m^2.g^{-1}$ for pure ceria to 105 $m^2.g^{-1}$ for the sample containing 2% of Cu, indicating the benefic role od the doping process on the textural properties.

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References

1. M. Dubey, S. Wadhwa, A. Mathur, R. Kumar, *Applied Surface Science Advances* vol. 12 100340 (2022).
2. Florea, M. F. Matei-Rutkovska, G. Postole, A. Urda, F. Neatu, V.I. Pârvulescu, P. Gelin, *Catal Today* 306, (2018).

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Doped TiO_2-SiO_2 as efficient photocatalysts

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Decontamination is a vital part of safe military operations, as it reduces the risk of contact and persistence. Standard decontamination involves applying a decontaminating agent to the contaminated surface, allowing the neutralization reactions to complete, and then physically removing the reaction products or the contaminant–decontaminant system. These procedures have numerous disadvantages (high consumption of materials, energy, and time; complex logistics; the need for trained and qualified personnel; significant environmental impact, etc.), which is why decontamination specialists have researched new methods based on completely different principles to at least partially eliminate them. Nowadays, NATO decontamination technologies improve efficiency and productivity compared to wet spraying/irrigation of decontamination solutions/suspensions or to dry processes (superheated steam). Experience in the field of CBRN protection has led to a new "philosophy" of decontamination that emphasizes neutralization, speed, materials, manpower, and environmental protection. For this purpose, we design materials based on TiO_2 and SiO_2 that possess all the properties to decontaminate efficiently under light on different surfaces. The materials were prepared by impregnation of TiO_2-SiO_2 prepared previously by the sol-gel method [1, 2], with salts of the doping elements such as vanadium and iron.

All prepared materials were fully characterized by using different techniques to determine textural (adsorption-desorption isotherms) and structural (X-ray diffraction, TG-DSC, FTIR, TPD-TPR-TPO, Raman, UV-VIS, XPS, particle size) properties to prove the reproducibility of the synthesis method at the laboratory scale.

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References
1. S. Neatu, V. I. Parvulescu, G. Epure, E. Preda, V. Somoghi, A. Damin, S. Bordiga, A. Zecchina, *Phys. Chem. Chem. Phys. 10 (43)*, 6562 (2008)
2. S. Neatu, V. I. Parvulescu, G. Epure, N. Petrea, V. Somoghi, S. Bordiga, G. Richiardi, A. Zecchina, *Appl. Catal. B*: Environ. *91 (1-2)*, 546 (2009).

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Bilateral cooperation Romania-Republic of Moldova for food safety: cross-border approach to microbiological risks in fresh meat traded

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Introduction. Food safety is a major public health concern, particularly in the context of the consumption of poultry meat, which is prone to contamination by zoonotic bacteria. Microbial contamination reflects hygiene conditions along the food chain as well as the misuse of antibiotics in animal production.

The objective of the study was to investigate the microbiological profile and antimicrobial resistance of bacteria isolated from refrigerated poultry meat and potential risks for public health.

Research material and methods. The experimental material was collected from commercial markets from c. Chisinau, Republic of Moldova. For bacteriological investigation were used the selective and differential culture media. For morphological indicators of bacterial colonials were notified size, color, mucoid/non-mucoid appearance. Bacterial identification was performed using MALDI-TOF mass spectrometry (Bruker Biotyper).

Results. A wide diversity of Gram-negative bacteria was isolated, with *Enterobacteriaceae* predominating. *Escherichia coli* and *Proteus mirabilis* were the most frequent isolates, followed by *Klebsiella spp., Citrobacter spp*., and *Morganella morganii*. The results highlighted a broad spectrum of colony appearances, reflecting a complex microflora which contaminated the samples. The detection of ESBL producing *Escherichia coli* and *Klebsiella pneumoniae/oxytoca* is consistent with global reports of poultry as a major ESBL reservoir. The isolation of *Escherichia coli* in intense blue colonies on ESBL agar underscores its dominance as both a commensal and a resistant pathogen. Another important point is antibiogram results showed frequent resistance to third-generation cephalosporins (ceftazidime), aztreonam, fluoroquinolones, and tetracyclines. Resistance to fluoroquinolones such as enrofloxacin is especially worrisome, since these antibiotics are still widely used in veterinary medicine and represent critical antimicrobials in human therapy. Thus, our findings from Moldova fit within a broader global pattern of poultry as a reservoir and amplifier of resistance genes.

Conclusions. This study demonstrated that refrigerated poultry meat sold in commercial markets from c. Chisinau, Republic of Moldova, harbors a diverse microbiota, dominated by *Escherichia coli, Proteus mirabilis, Klebsiella spp.*, and *Citrobacter spp.*, alongside opportunistic non-fermenters such as *Pseudomonas aeruginosa* and *Acinetobacter pittii*. The repeated detection of ESBL-producing Enterobacteriaceae, particularly *Escherichia coli* and *Klebsiella pneumoniae*, highlights poultry meat as an important reservoir of antimicrobial resistance genes with zoonotic potential.

Keywords: poultry meat; microorganisms; antimicrobial resistance; bacterial colonies.

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The role of polyphenols extracted from green walnuts in the prophylaxis of oxidative stress in male rabbits

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Under the influence of various internal or external factors, the decrease in proliferative potential is conditioned due to reactions caused by reactive oxygen species, which are formed as a result of energy metabolism in mitochondria, microsomes and other specialized cells and systems, where the main source is the reduction of oxygen performed by mitochondria.Oxidative stress justifies the basic role in the pathogenesis of diminishing the functions of the body's systems and determines the need to use antioxidants to maintain the body's homeostasis. At the cellular and tissue level, oxidative stress manifests various homeostatic disorders: endothelial dysfunction, hypoxia, dysregulation of amino acid metabolism, energetic and metabolic disorders, disorders of telomerase activity of cellular chromosomes. The accumulation in the cell of the suboxidized products, formed as a result of protein and lipid degradation, leads to pronounced disorders of the cellular redox potential (oxidation-reduction potential in cell membranes), which disrupts the processes of penetration into the cells of the organism of substances necessary for normal functioning and the elimination of disintegrated products. In our laboratory, research was conducted dedicated to studying the influence of polyphenols extracted from green walnuts on changes in antioxidant status in male rabbits. To achieve this goal, hydroalcoholic extracts were obtained from green walnuts. The extract was administered to breeding rabbits at a dose of one milliliter per animal, with a total polyphenol content of 548.37 mg/100g gallic acid equivalent (GAE). The research results are presented in the table below.

Biochemical indices in the blood serum of breeding rabbits

Groups	GST, nM/L	Phosphorus, mM/L	Mg, mM/L	Total protein, g/L
Control	16,53±0,15	1,47±0,14	0,760±0,11	71,2±1,21
Experimental	22,1±0,32	1,7±0,18	0,840±0,18	74,7±1,46

From the results obtained, we observe that glutamate-S-transferase, being part of the fermentative antioxidant status, is influenced by polyphenols extracted from green walnuts, which demonstrates that at the administration of this extract the amount of this ferment increases by approximately 21% in the experimental group. Phosphorus and magnesium, being elements of the mineral antioxidant status, also undergo increasing changes, namely for phosphorus a difference of 0.23 mM/L is observed. Phosphorus compounds play an important role in energy metabolism (ATP and creatine phosphate are energy accumulators that provide many processes in the body with energy). Magnesium is also a macroelement that participates in the processes of energy synthesis, is an active participant in the synthesis of proteins, phospholipids of cell membranes, stabilizing their fluidity and permeability. It is an active regulator of cholesterol content in the blood, improves blood circulation in the parenchymal tissues of the body, including the testicles. Magnesium values showed a difference of 0.08 mM/L between the control and experimental groups. Total protein is part of the major components of the organism, performing a multitude of functions to maintain a huge diversity of biochemical reactions in all systems of living organisms, manifesting itself through the regulation of metabolic activity, catalyzing biochemical reactions, serves as a plastic material for all cells and tissues of the organism. Proteins participate in the synthesis of enzymes, hormones and antibodies, which are included in the functioning of the antioxidant system. Proteins are also responsible for maintaining acid-base balance (pH) and are also a source of energy. In the researches carried out in our laboratory, we obtained a value for the control group of 71.2±1.21 g/L and for the experimental group of 74.7±1.46 g/L. Finally, we can conclude that polyphenols extracted from green walnuts have an influence on the antioxidant system, favoring extracellular, transmembrane and intracellular metabolic processes, through the neutralization of free radicals and the detoxification of body cells.

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